

National Aeronautics and
Space Administration



HIGH-END COMPUTING CAPABILITY PORTFOLIO

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NASA Advanced Supercomputing Division

August 10, 2021

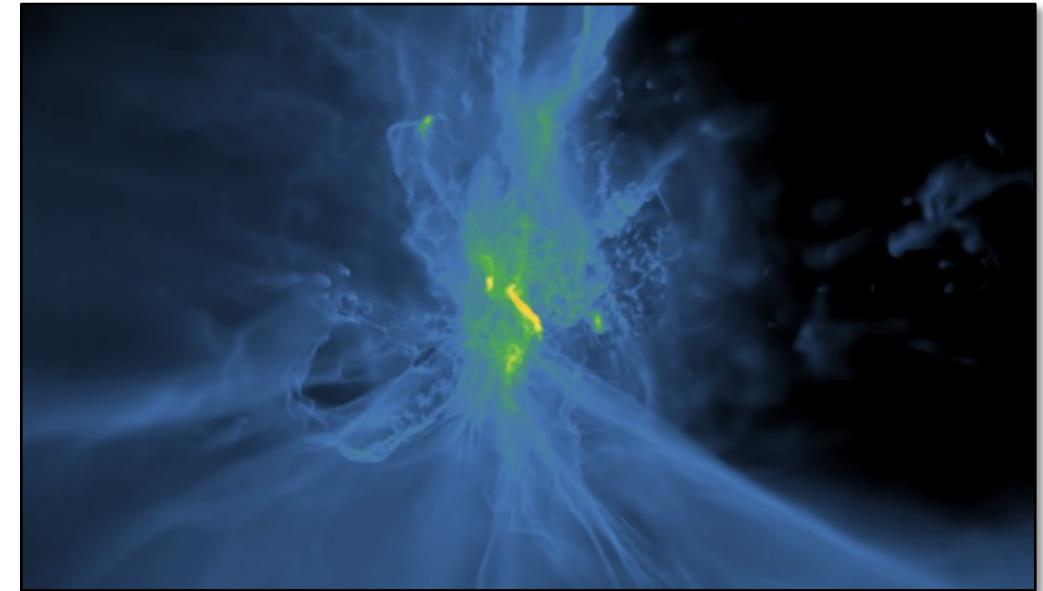


HECC Supercomputer Usage Sets New Record

- In July, the combined usage of HECC supercomputers set a new record of 12,338,448 Standard Billing Units (SBUs).*
- The usage by 425 of NASA's science and engineering groups exceeded the previous record of 11,662,724 SBUs set in March 2021 by 675,724 SBUs (6%).
- The record was achieved in great part by the Science Mission Directorate's Earth Science group from a coupled study of Goddard Earth Observing System (GEOS)/Estimating the Circulation and Climate of the Ocean (ECCO).
- Usage of Pleiades, Aitken, Electra, and Endeavour contributed to this record.
- The top 10 projects' usage ranged between 209,787 and 1,156,813 SBUs per project and together accounted for over 33% of the total usage.
- Additional expansions to Aitken are underway and will be online in November and January.

* 1 SBU represents the work that can be done in 1 hour on a Pleiades Broadwell 28-core node.

IMPACT: Both the increased capacity of HECC systems and support work with users to optimize their run capacities provide mission directorates with more resources to accomplish their goals and objectives.

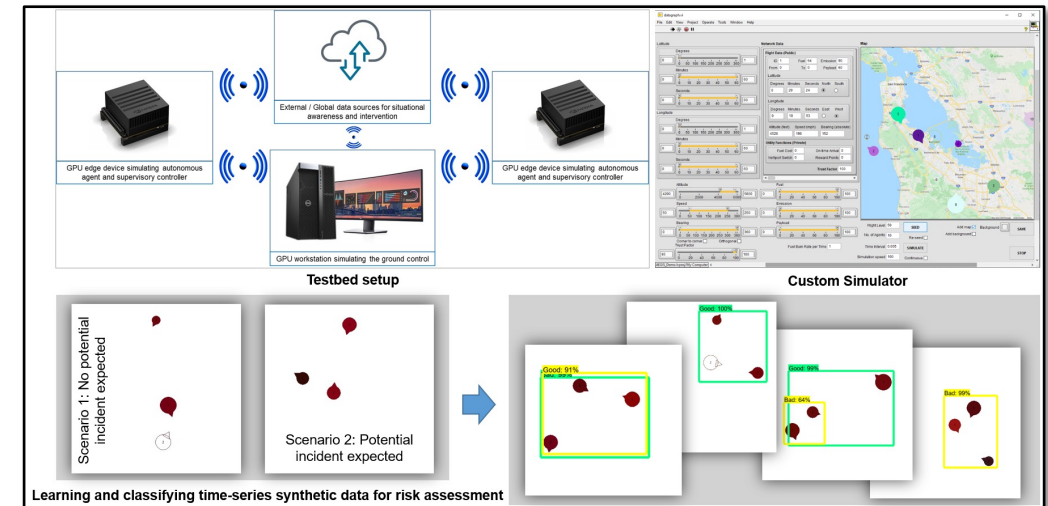


Snapshot of a visualization showing gas in and around a simulated galaxy. The simulation was run by the Figuring Out Gas & Galaxies In Enzo (FOGGIE) project using the Enzo cosmological hydrodynamic code. *Raymond Simons, Space Telescope Science Institute (STScI); Molly S. Peeples, STScI/Johns Hopkins University*

New Machine Learning Sandbox Available on AWS Cloud

- HECC's Data Science team began a pilot effort for a machine learning (ML) capabilities sandbox, created for the HECC Amazon Web Services (AWS) Cloud with NASA Enterprise Managed Cloud Computing (EMCC) Service authorization. The capabilities are scheduled to go into production in fall 2021.
 - The sandbox agreement with EMCC to allow AWS artificial intelligence(AI)/ML services was used for the pilot efforts.
 - The Data Science team completed SageMaker service testing and resolved initial issues with roles, access, storage, and endpoints.
 - AWS accounts have been configured to allow accounting/billing without PBS.
- Two teams from NASA's Digital Transformation AI/ML thrust are currently using the sandbox for AWS AI/ML access through September 2021. Work includes:
 - Transition the on-premise implementation of the AEGIS framework to the cloud with secure web access for data I/O.
 - Integrate satellite, surface, and model outputs into a machine learning algorithm to forecast air quality during fire season.
 - Integrate surface, satellite, and model outputs into ML-ready datasets in a cloud environment.
 - Develop a prototype machine learning algorithm to forecast air quality during agriculture burning.

IMPACT: Adding artificial intelligence/machine learning capabilities to the HECC AWS cloud offering provides tools and capabilities available on the AWS platform to NASA users.

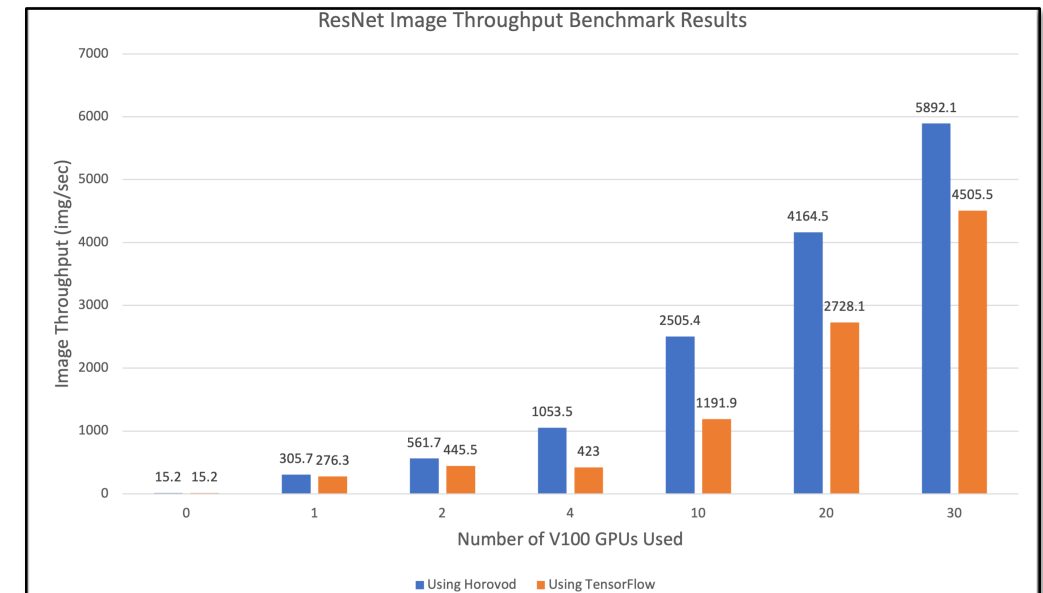


The AWS machine learning capability as proposed by Aditya Das (NASA Ames), in the NASA Technical Memorandum, “Autonomous Entity Global Intelligence System (AEGIS).”

HECC Supports Multi-Node GPU Training with Horovod

- The HECC Data Science team added support for use of TensorFlow's Horovod framework for multi-node GPU machine learning model training. Advantages of using Horovod:
 - Allows for easy distribution of training to multiple nodes.
 - Uses MPI to communicate between nodes.
 - Is thirty percent faster than TensorFlow's built in multi-node distribution, which uses Google's remote procedure call (gRPC) to communicate between nodes.
 - After code changes are applied, is easy to scale to any number of nodes to determine the optimal number.
 - Can process over 10 times more images by distributing training from 1 node to 15 nodes (2 GPUs each).
- The team studied scaling efficiency for image throughput on multiple GPUs across multiple nodes relative to a single GPU.
 - Scaling efficiency per node drops from 91% on 1 node (2 GPUs) to 64% on 15 nodes (30 GPUs) due to distribution.
 - Wall time was kept the same at 1 minute for all runs.
- The framework can be easily accessed through the team's conda module and environment; more information is available here: https://www.nas.nasa.gov/hecc/support/kb/machine-learning-overview_572.html

IMPACT: HECC support for distributed, multi-GPU machine learning model training using the Horovod framework enables scaling for performance and provides increased throughput for training with large datasets.

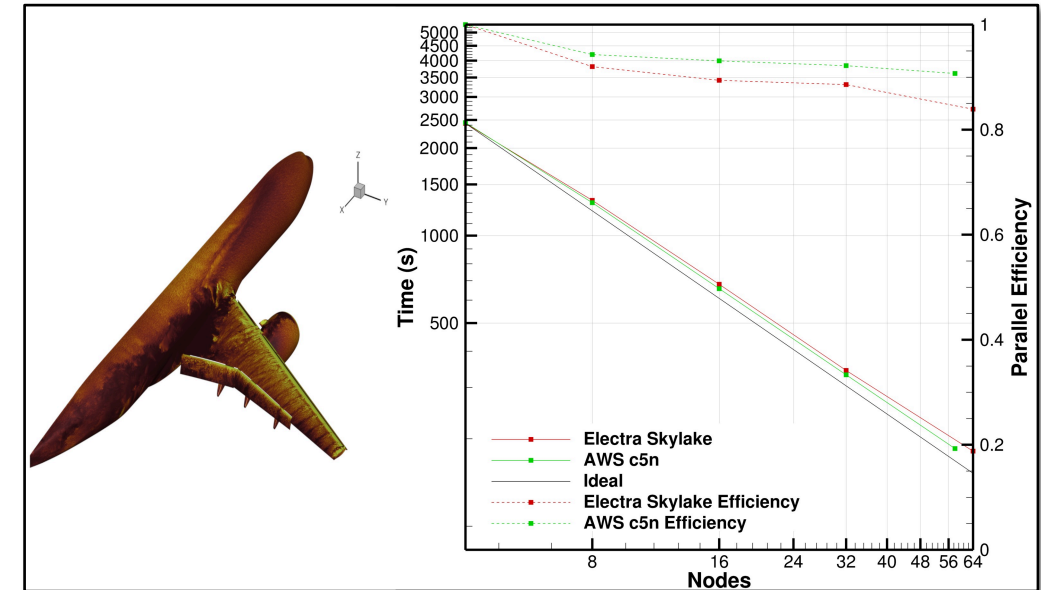


Throughput comparison of a ResNet Benchmark using Horovod and TensorFlow. 0 GPUs is running only on Cascade Lake CPUs.
HECC Data Science Team

LAVA Team Successfully Performs Production Simulations Using HECC Cloud Resources

- With support from HECC Cloud staff, the Launch Ascent and Vehicle Aerodynamics (LAVA) team recently performed production scale-resolving simulations using Amazon Web Services (AWS) cloud resources.
 - The test case is a Wall-Modeled Large Eddy Simulation (WMLES) with NASA's High-Lift Prediction workshop grid consisting of ~400M points.
 - The code was compiled on Pleiades with the Intel Message Passing Library and the executable was then transferred to AWS.
 - The LAVA team used AWS c5n nodes (Intel Skylake) connected with Amazon's high-performance Elastic Fabric Adapter (EFA). They compared the performance to HECC's Skylake nodes connected with InfiniBand.
 - The team found that no tweaking was required for excellent performance. Runs achieved greater than 90% parallel efficiency on 58 nodes— better scaling than on-premises runs.
- For a suite of runs using 4-64 nodes, the compute-only cost was:
 - \$34.39 using AWS “on-demand” resources.
 - \$ 7.42 on premises at HECC (using \$0.47/SBU as the rate).
 - Using “spot” pricing at AWS would cut the cost in half but would introduce a risk that resources could be taken away mid-job.
 - The on-premises average wait time for a HECC job is 31.5 hours. AWS “on-demand” has no wait time.
- The LAVA team now plans to investigate high-cadence I/O for large-scale post-processing visualizations.

IMPACT: Demonstrating cloud capabilities beyond traditional on-premises high-performance computing resources helps HECC meet the ever-increasing demand of various scientific and engineering requirements within the agency.

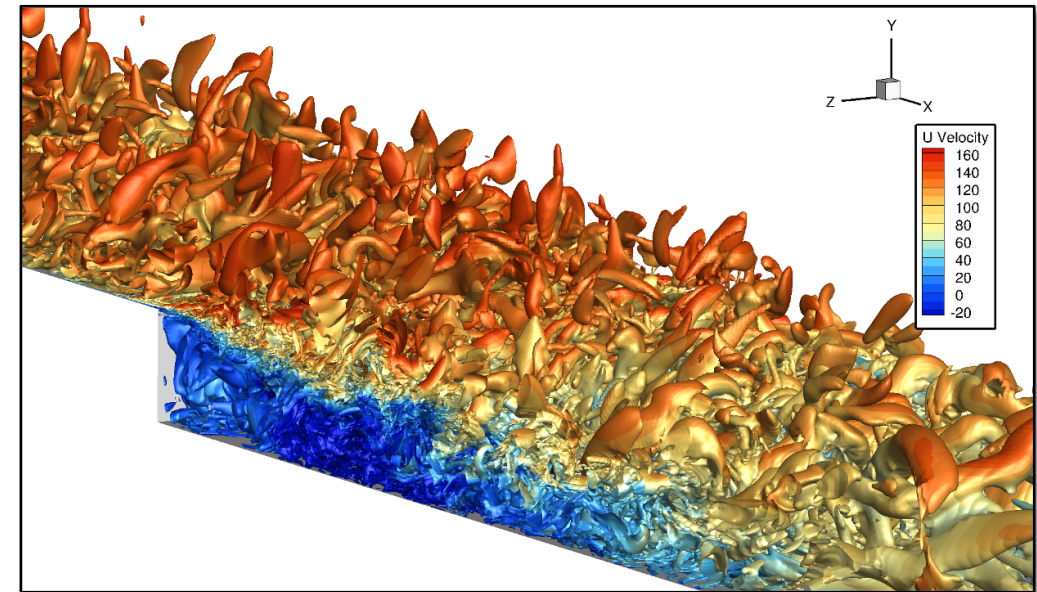


Performance comparison of the Wall-Modeled Large Eddy Simulations (WMLES) on Amazon Web Services (AWS) c5n and Electra Skylake nodes, with the High-Lift Prediction Workshop grid.
Gaetan Kenway, Aditya Ghate, NASA Ames

Application Experts Improve Performance of Large-Eddy Simulation Code

- HECC's Application Performance and Productivity (APP) team recently improved the performance of the Wave-Resolving Large-Eddy Simulation (WRLES) code by 30%.
 - WRLES is a high-fidelity Navier-Stokes solver designed for scale-resolving simulations of turbulent flows with application to air-breathing propulsion concepts. WRLES is being developed at NASA Glenn.
 - The simulations performed on HECC resources are focused on improving predictions of separated and free shear flows, with the end goal of reducing noise during aircraft takeoff and landing or improving the fuel efficiency of commercial aircraft during all stages of flight.
- The APP team used Supersmith's op_scope tool to locate performance bottlenecks and then addressed the issues causing each bottleneck.
 - The optimization technique most responsible for improving performance is the application of OpenMP directives that enable parallel access to numerous arrays.
 - The modified code is currently being used for production simulations.
- In addition, the APP team searched WRLES for latent bugs. That investigation led the code developer to find and fix an issue that might have impacted numerical results.

IMPACT: HECC's improved performance of WRLES can be used to extend the duration or increase the fidelity of simulations. In either case, the user is able to get more done with the limited resources that are currently available.



Large eddy simulation of the Driver-Seegmiller backward-facing step Q-Criterion isosurfaces colored by axial velocity.

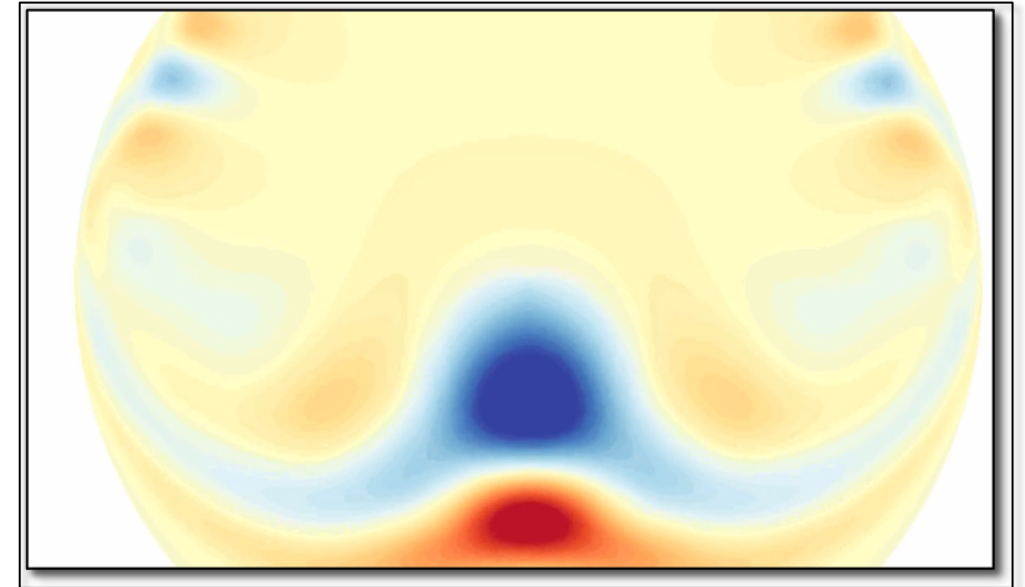
James DeBonis, NASA/Glenn

Predicting Jet Noise for Full-Scale Low-Boom Aircraft *

- To gain deeper insight into the nature of meridional flows throughout the solar interior, researchers at New Jersey Institute of Technology (NJIT) ran helio-physics simulations for thousands of CPU-hours on Pleiades. These velocity fields play a key role in distributing magnetic flux and regulating the 11-year period observed in the Sun's magnetic cycle.
 - The NJIT stellar models use new pseudo-spectral computational techniques to capture the impacts of internal velocities on the propagation of sound waves.
 - By simulating various models of internal flows, they can test techniques in local helioseismology that can offer critical insights on the data inferred from the Sun.
- These global 3D simulations allow exploration of the functional differences that many competing theories create and offer a basis for identifying the subtle changes in structures that inform our understanding of solar observations.
- The team continues using their model to test increasingly complex systems of internal solar dynamics, to aid in developing functional prediction techniques for magnetic events on the solar surface.

* HECC provided supercomputing resources and services in support of this work

IMPACT: These numerical simulations, enabled by HECC resources, have become critical foundational tools in physics and will help researchers continue to answer questions integral to our understanding of the universe.

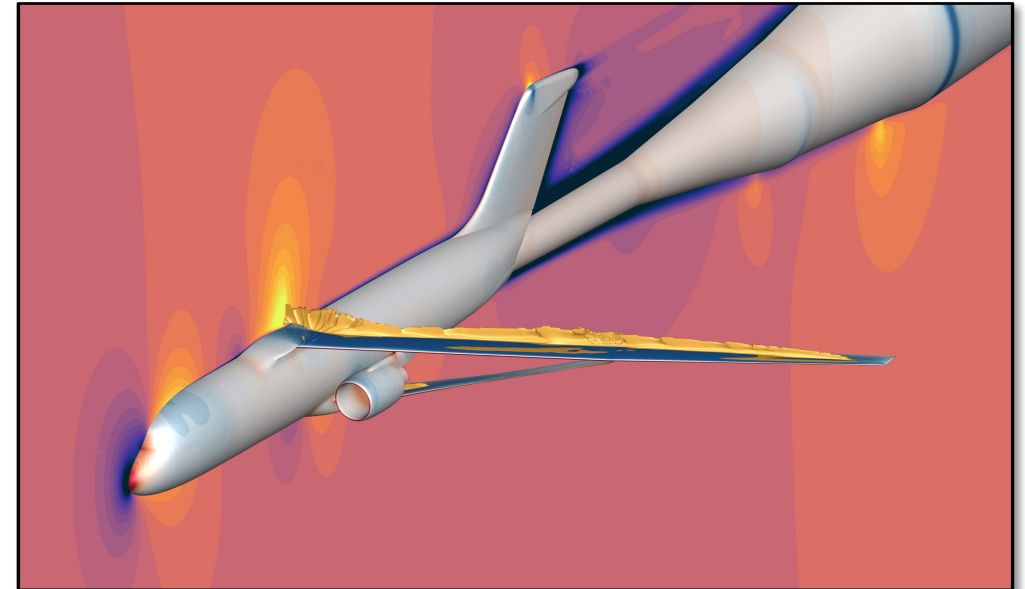


Video showing how a sound wave travels through the interior of the Sun. Increasing gas density strongly results in an increasing sound speed, shown by how the wave front accelerates as it goes deeper toward the core. *Andrey Stejko, Alexander Kosovichev, New Jersey Institute of Technology*

Best Practices for Transonic Truss-Braced Wing Modeling *

- The Transonic-Truss Braced Wing (TTBW) aircraft concept is part of a joint NASA/Boeing effort to develop advanced subsonic commercial transport vehicles to meet agency goals of reduced aircraft noise, emissions, and fuel consumption. Due to the complexity of the configuration, new computational fluid dynamics (CFD) best practices were developed by researchers from NASA's Langley and Ames Research Centers in order to accurately predict aircraft performance using the in-house USM3D software and Launch Ascent and Vehicle Aerodynamics (LAVA) framework.
- Initial efforts for best practices involved a code-to-code verification process simulating the flight configuration and a validation comparison against experimental results from the Ames 11-by-11-foot Transonic Wind Tunnel.
- Recently, simulations of the Mach 0.8 TTBW variant focused on minimizing differences between experimental data and computational predictions where possible. LAVA simulations included angle-of-attack sweeps for flight and wind tunnel configurations, grid refinement studies, and component build-ups to determine the influence each one has on the vehicle performance.
- The in-tunnel simulations using the production version of LAVA required eight days and 14 hours across 400 Ivy Bridge cores on Pleiades, while a refactored version of LAVA was able to run simulations double the size on 1,000 cores over 12 hours—a 12x reduction in resource cost.

IMPACT: Ensuring best practices for computational fluid dynamics simulations for aircraft design, prediction, and validation increases confidence in the accuracy of computational methods, which will help to reduce the cost of time and resources in the development of new aircraft.



Visualization of shock location over the wing for a free air simulation of the wind tunnel configuration, showing pressure coefficient contours over the surface of the model and Mach number on the symmetry plane. *Daniel Maldonado, Jeffrey Housman, NASA/Ames*

* HECC provided supercomputing resources and services in support of this work

Papers

- **“Performance of Wall-Modeled LES with Boundary-Layer-Conforming Grids for External Aerodynamics,”** A. Lozano-Duran, S. Bose, P. Moin, arXiv:2107.01506 [physics.flu-dyn], July 3, 2021. *
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<https://link.springer.com/article/10.1007/s41115-021-00012-0>
- **“TOI-2076 and TOI-1807: Two Young, Comoving Planetary Systems within 50 pc Identified by TESS that are Ideal Candidates for Further Follow Up,”** C. Hedges, et al., The Astronomical Journal, vol. 162, no. 2, July 12, 2021. *
<https://iopscience.iop.org/article/10.3847/1538-3881/ac06cd/meta>
- **“Dark Primitive Asteroids Account for a Large Share of K/Pg-Scale Impacts on the Earth,”** D. Nesvorný, W. Bottke, S. Marchi, Icarus, vol. 368, published online July 15, 2021. *
<https://www.sciencedirect.com/science/article/abs/pii/S0019103521002840>
- **“Stellar Wind Confinement of Evaporating Exoplanet Atmospheres and its Signatures in 1083 nm Observations,”** M. MacLeod, A. Okločić, arXiv:2107.07534 [astro-ph.EP], July 15, 2021. *
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* HECC provided supercomputing resources and services in support of this work

Papers (cont.)

- **“Scaling Out Transformer Models for Retrosynthesis on Supercomputers,”** J. Mollinga, V. Codreanu, Intelligent Computing: Lecture Notes in Networks and Systems, vol. 283, published online July 13, 2021. *
https://link.springer.com/chapter/10.1007/978-3-030-80119-9_4
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- **“Sgr A* X-ray Flares from Non-Thermal Particle Acceleration in a Magnetically Arrested Disc,”** N. Scepi, J. Dexter, M. Begelman, arXiv:2107.08056 [astro-ph.HE], July 16, 2021. *
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Papers (cont.)

- **“Large-Scale Structure and Turbulence Transport in the Inner Solar Wind – Comparison of Parker Solar Probe’s First Five Orbits with a Global 3D Reynolds-Averaged MHD Model,”** R. Chhiber, et al., arXiv:2107.11657 [physics.space-ph], July 24, 2021. *
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- **AIAA Aviation 2021 Forum**, Virtual Event, August 2-6, 2021, published online July 28, 2021.
 - **“Airframe Noise Simulations of a Full-Scale Large Civil Transport in Landing Configuration,”** M. Khorrami, et al. *
<https://arc.aiaa.org/doi/abs/10.2514/6.2021-2161>
 - **“Aeroacoustic Study of a Subscale Large Civil Transport (STAR) Model – Part 1: Simulations,”** B. Koing, et al. *
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Papers (cont.)

- **AIAA Aviation 2021 Forum (cont.)**

- **“Aeroacoustic Computations of a Generic Low Boom Concept in Landing Configuration: Part 1 – Aerodynamic Simulations,”** R. Ferris, et al. *
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- **“Multiplanar Synthetic Arrays and their Application to Full-Scale Landing Gear Noise Source Identification,”** P. Ravetta, et al. *
<https://arc.aiaa.org/doi/abs/10.2514/6.2021-2163>
- **“Coupled Aeropropulsive Design Optimization of a Podded Electric Propulsor,”** A. Yildirim, et al. *
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- **“Hypersonic Boundary-Layer Transition on Blunted Cones at Angle of Attack,”** P. Paredes, et al. *
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- **“Full-Envelope Aero-Propulsive Model Identification for Lift+Cruise Aircraft Using Computational Experiments,”** B. Simmons, et al. *
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- **“Effect of Geometric Granularity on the Noise Signature of a Full-Scale Large Civil Transport Nose,”** E. Fares, et al. *
<https://arc.aiaa.org/doi/abs/10.2514/6.2021-2134>

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Papers (cont.)

- **AIAA Aviation 2021 Forum (cont.)**

- **“Design Exploration of a Transonic Cruise Slotted Airfoil,”** B. Hiller, et al. *
<https://arc.aiaa.org/doi/abs/10.2514/6.2021-2525>
- **“Comparison of Boeing 777 Airframe Noise Flight Test Data with Numerical Simulations,”** M. Czech, et al. *
<https://arc.aiaa.org/doi/abs/10.2514/6.2021-2162>
- **“Efficient Preconditioning of a High-Order Solver for Multiple Physics,”** M. Franciolini, et al. *
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- **“Integral Velocity Sampling for Unsteady Rotor Models on Cartesian Meshes,”** J. Chiew, M. Aftosmis. *
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- **“Unsteady Pressure-Sensitive-Paint Shot Noise Reduction,”** L. Tang, et al. *
<https://arc.aiaa.org/doi/abs/10.2514/6.2021-2579>
- **“Comparing Simulation Results from CHARM and RotCFD to the Multirotor Test Bed Experimental Data,”** S. Conley, D. Shirazi. *
<https://arc.aiaa.org/doi/abs/10.2514/6.2021-2540>
- **“Flow Characterization of the NASA Langley Unitary Plan Wind Tunnel, Test Section 2: Computational Results,”** R. Childs, et al. *
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- **“Adjoint-Based Minimization of X-59 Sonic Boom Noise Via Control Surfaces,”** D. Rodriguez, et al. *
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- **“Numerical Simulation of Lean Blowout of Alternative Fuels in 7-Element Lean Direct Injector,”** M. Endo, et al. *
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Papers (cont.)

- **AIAA Aviation 2021 Forum (cont.)**
 - **“Lean Blowout Predictions of a 7-Point Swirler-Venturi Lean Direct Injector Array from Large-Eddy Simulations,”** F. Guzman, et al. *
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 - **“Transition Analysis for Isolated Trips on BOLT-II Wind-Tunnel and Flight Configurations,”** F. Li, et al. *
<https://arc.aiaa.org/doi/abs/10.2514/6.2021-2905>
 - **“Axisymmetric and Asymmetric Turbulent Shockwave Boundary Layer Interaction at Mach 2.5,”** J.-P. Mosele, et al. *
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 - **“CFD Analysis of Space Launch System Solid Rocket Booster Separation with the Langley Unitary Plan Wind Tunnel,”** J. Koch, et al. *
<https://arc.aiaa.org/doi/abs/10.2514/6.2021-2966>
 - **“Evaluation of CFD Predictions of Cobra-MRV Control Surface Effectiveness at the NASA Langley Unitary Plan Wind Tunnel,”** M. Denison, et al. *
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Papers (cont.)

- **“HD 183579b: A Warm Sub-Neptune Transiting a Solar Twin Detected by TESS,”** T. Gan, et al., arXiv:2107.14015 [astro-ph.EP], July 29, 2021. *
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- **“TOI-1634 b: An Ultra-Short-Period Keystone Planet Sitting Inside the M-Dwarf Radius Valley,”** R. Cloutier, et al., The Astronomical Journal, vol. 162, no. 2, July 30, 2021. *
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News and Events

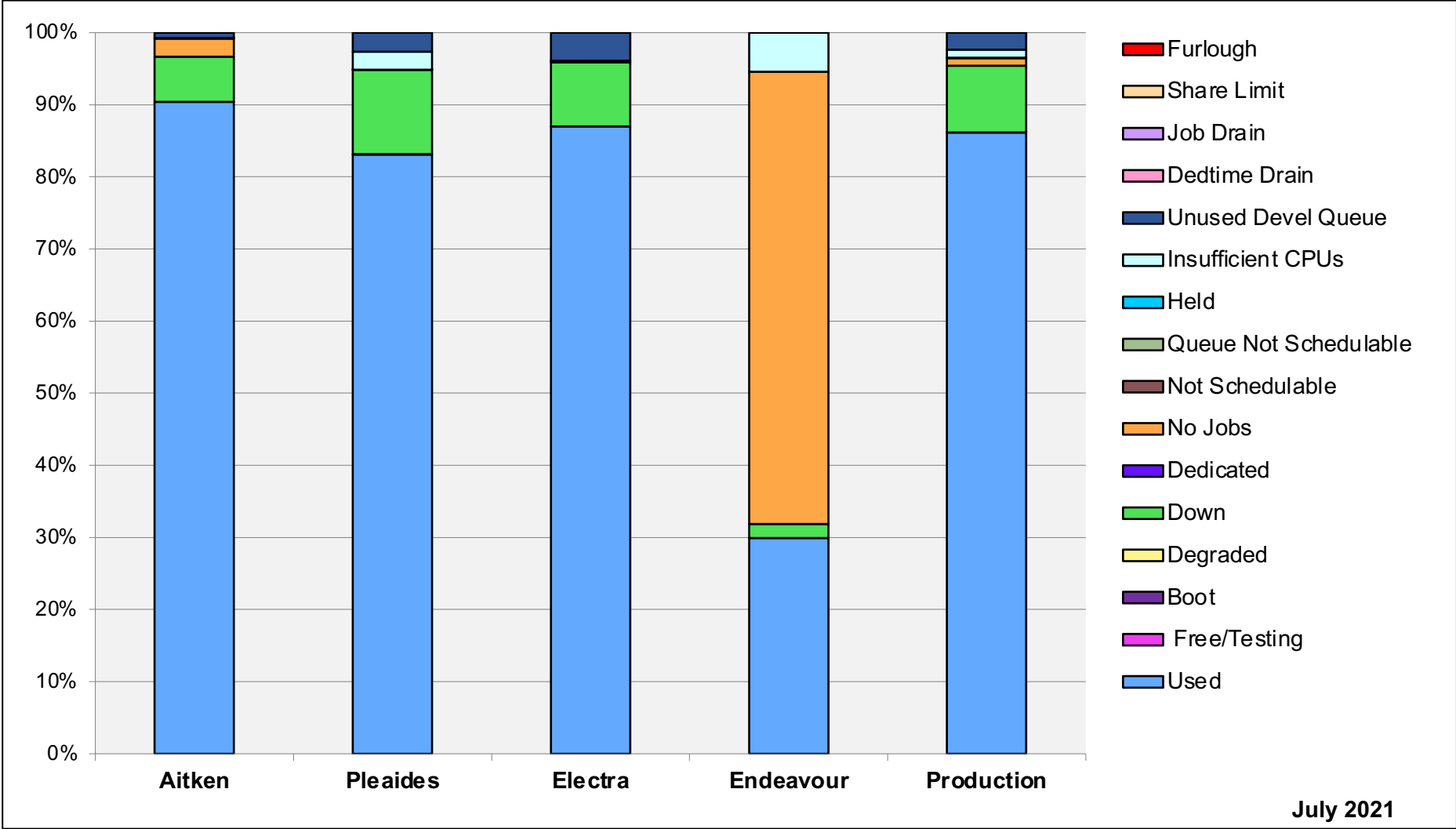
- **New Maps Help Developers Plan Lunar Road Trip for VIPER's Artemis Mission**, *NASA Ames*, July 15, 2021—A team at NASA's Ames Research Center is using the processing power of the Pleiades supercomputer, combined with NASA's open-source Stereo Pipeline software, to develop maps of the Moon's terrain by layering thousands of satellite images taken by cameras aboard the Lunar Reconnaissance Orbiter. The maps will be used by the Volatiles Investigating Polar Exploration Rover (VIPER), scheduled to land on the Moon in 2023 to search for ice and other resources.
<https://www.nasa.gov/feature/ames/new-maps-help-viper-plan-lunar-road-trip>
- **SwRI TEAM ZEROES IN ON SOURCE OF THE IMPACTOR THAT WIPED OUT THE DINOSAURS**, *SwRI*, July 27, 2021—Researchers from the Southwest Research Institute have used NASA's Pleiades supercomputer to simulate the evolutionary processes that deliver large asteroids to Earth from the outer half of the asteroid belt—a process now known to occur 10 times more frequently than previously thought.
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News and Events: Social Media

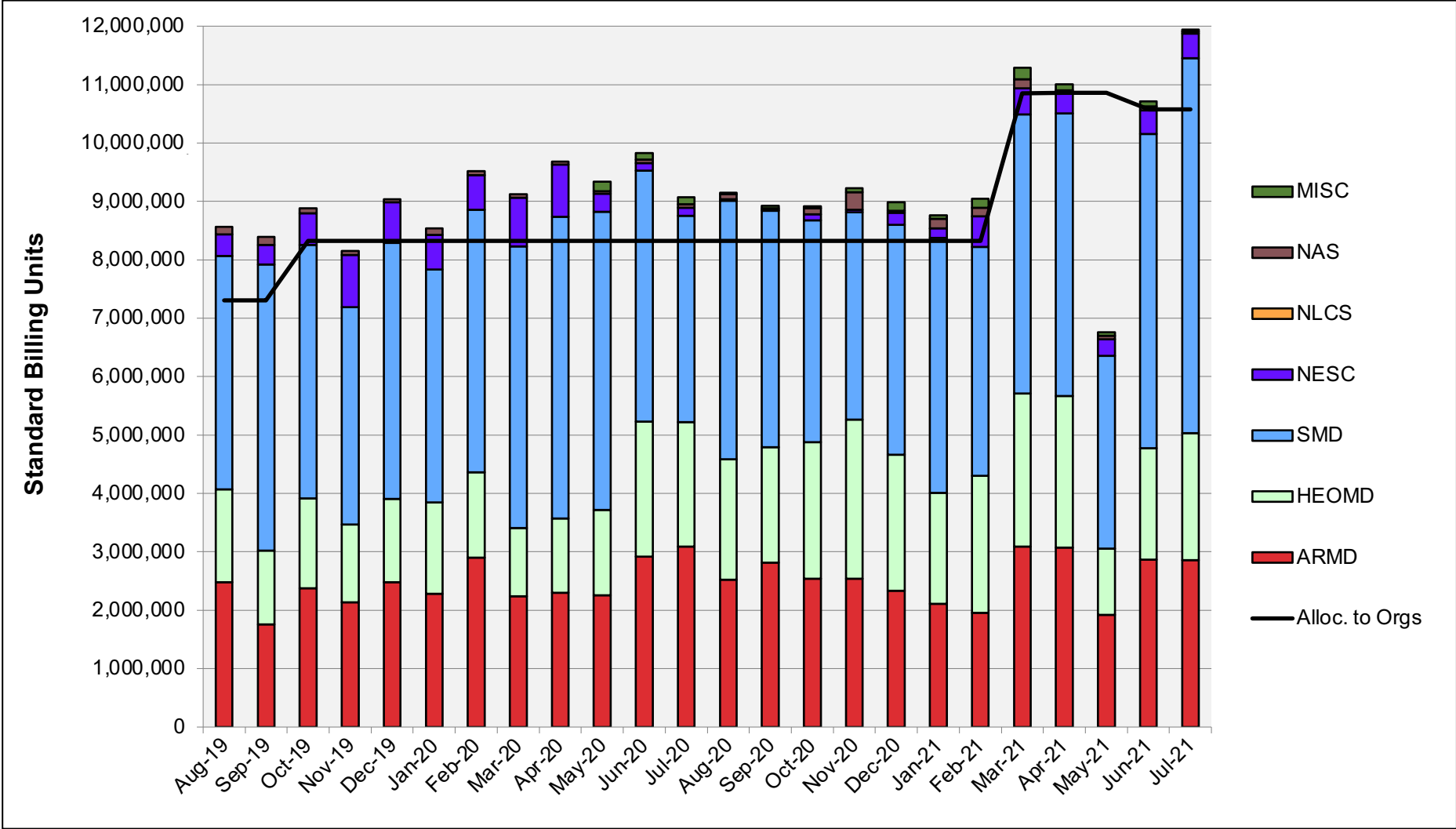
- **Coverage of NAS Stories**

- Asteroid impact simulations (Asteroid Day Campaign)
 - NAS: [Twitter](#) 2 retweets, 6 favorites.
 - NASA Supercomputing: [Facebook](#) 175 users reached, 19 engagements, 10 likes, 4 shares.
 - NASA Ames: [Facebook](#) 52 likes, 9 comments, 18 shares; [Twitter](#) 31 retweets, 1 quote tweet, 107 likes.
- Orion Crew Vehicle feature (throwback)
 - NAS: [Twitter](#) 1 retweets, 6 favorites.
 - NASA Supercomputing: [Facebook](#) 498 users reached, 78 engagements, 16 likes, 8 shares.
- Orion Launch Abort System installed
 - NASA Ames: [Facebook](#) 60 likes, 11 shares; [Twitter](#) 42 retweets, 2 quote tweets, 390 likes.
 - NASA Supercomputing: [Facebook](#) 460 users reached, 20 engagements, 12 likes 2 shares.

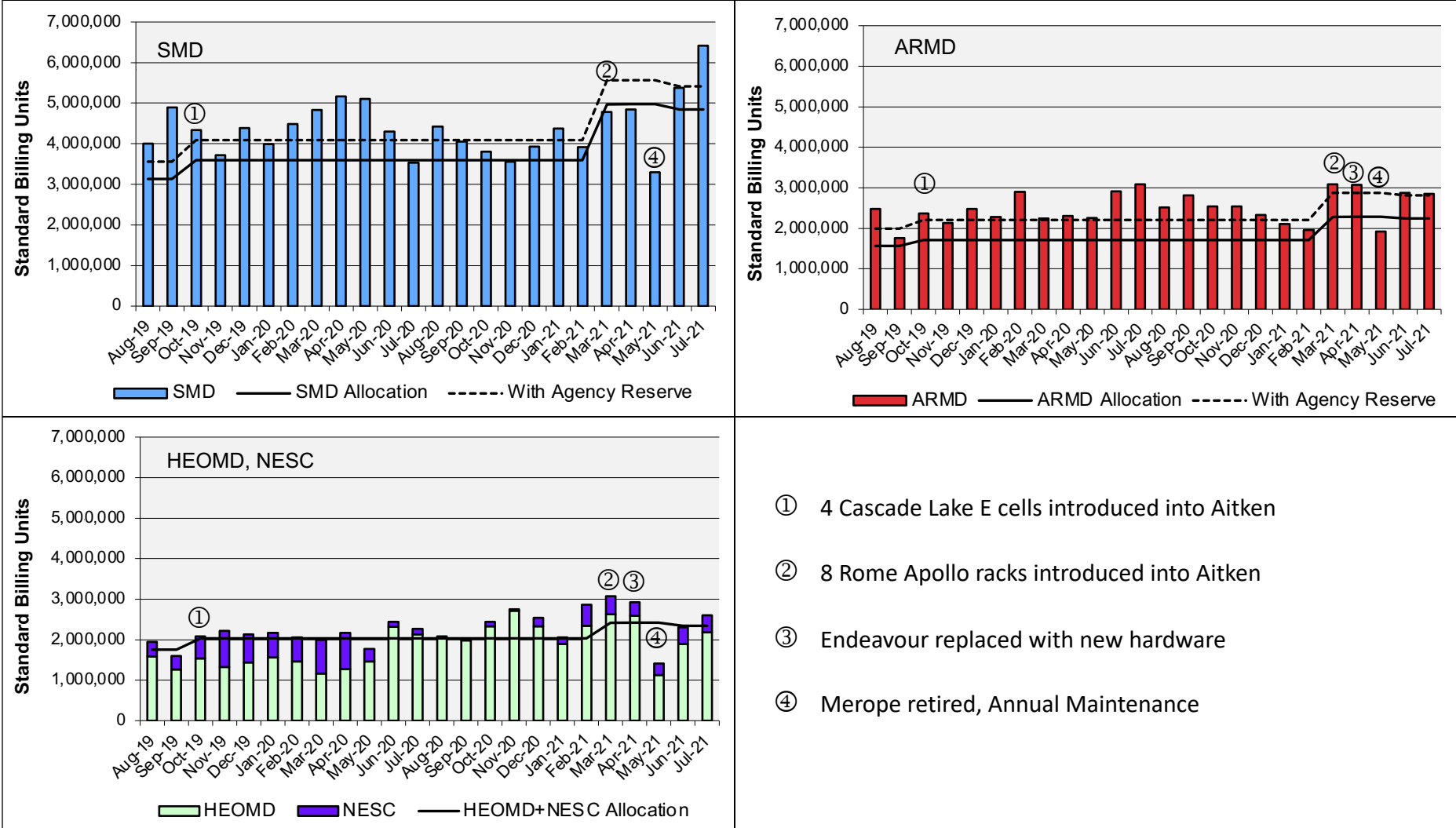
HECC Utilization



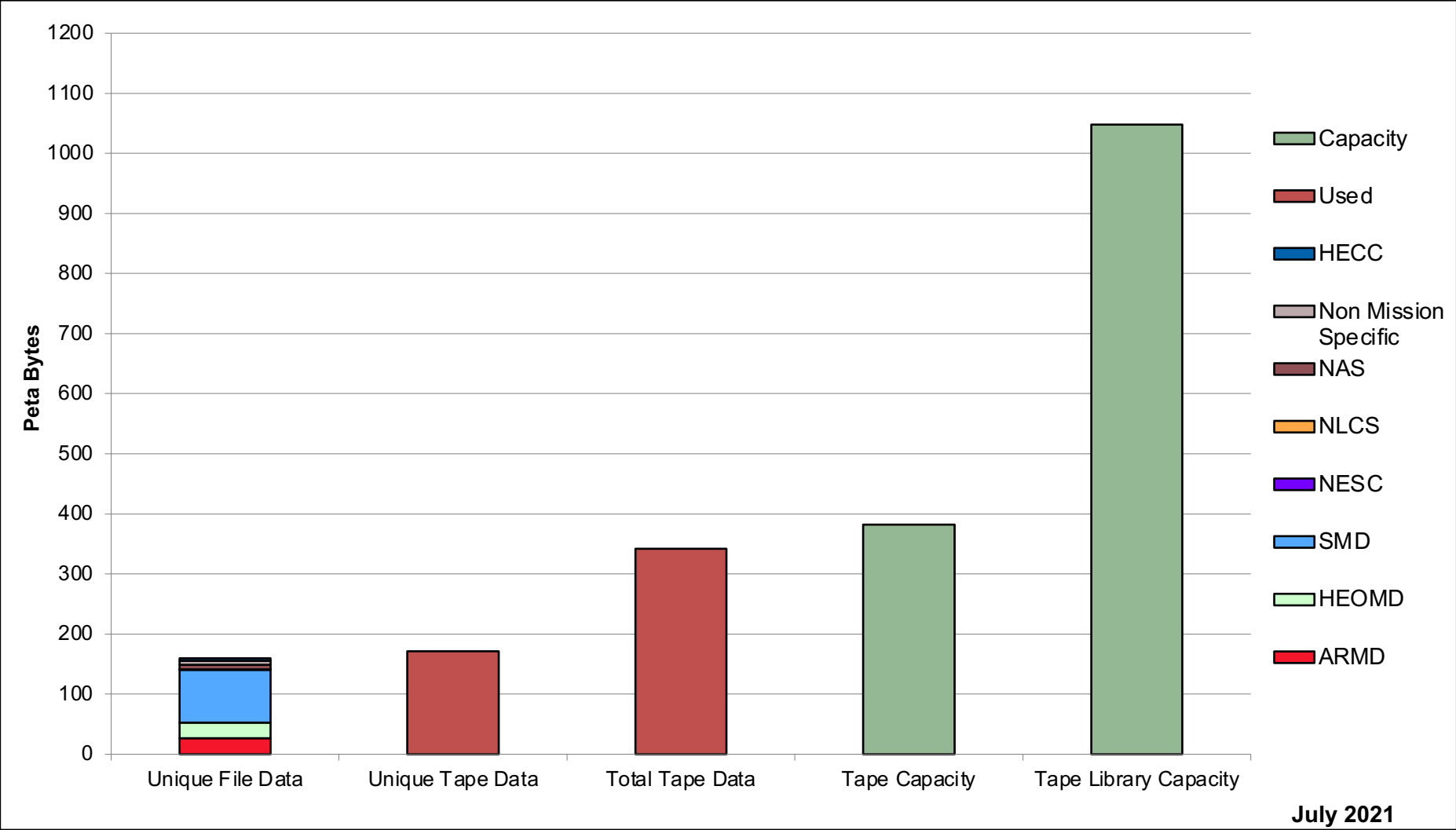
HECC Utilization Normalized to 30-Day Month



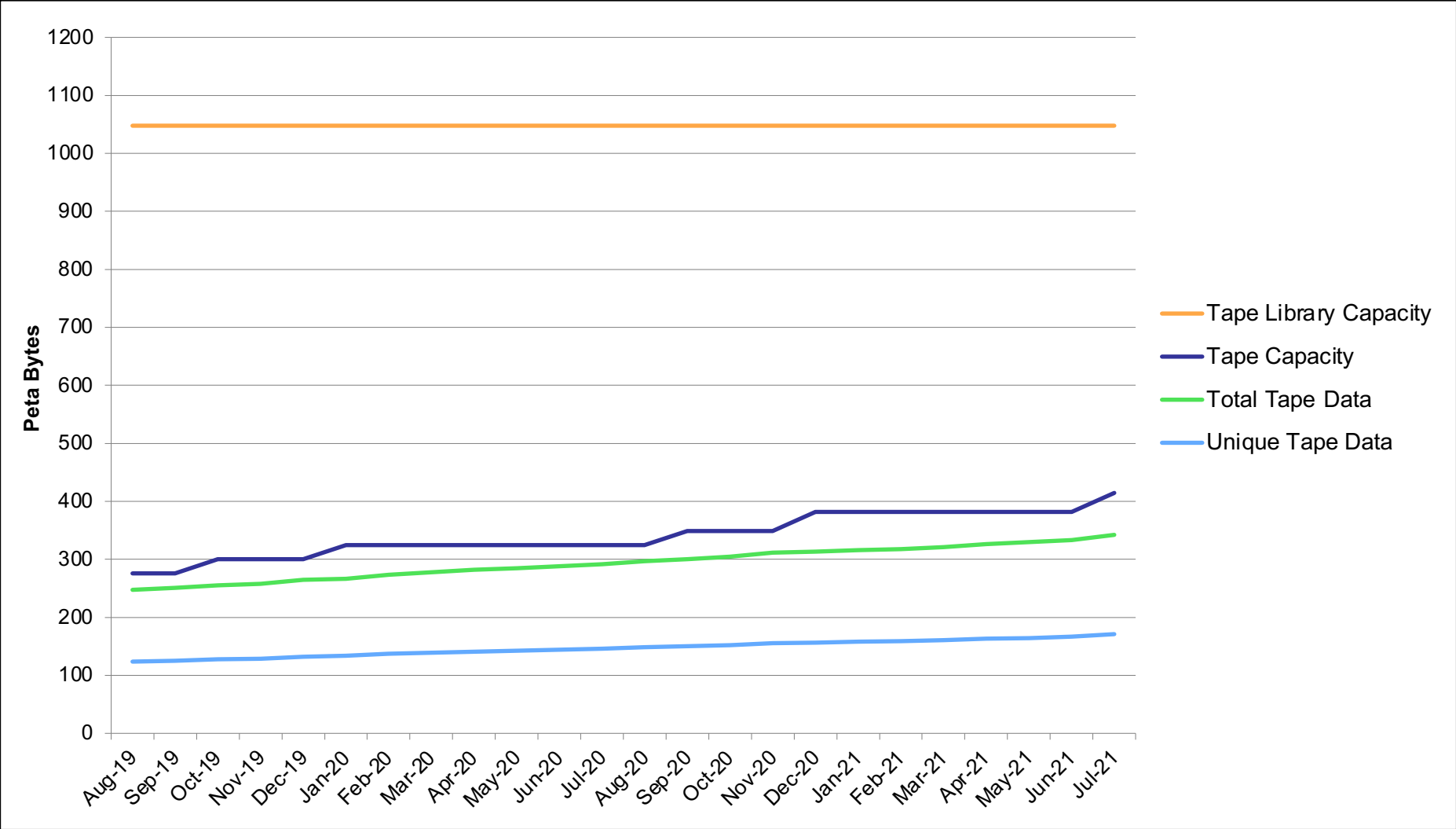
HECC Utilization Normalized to 30-Day Month



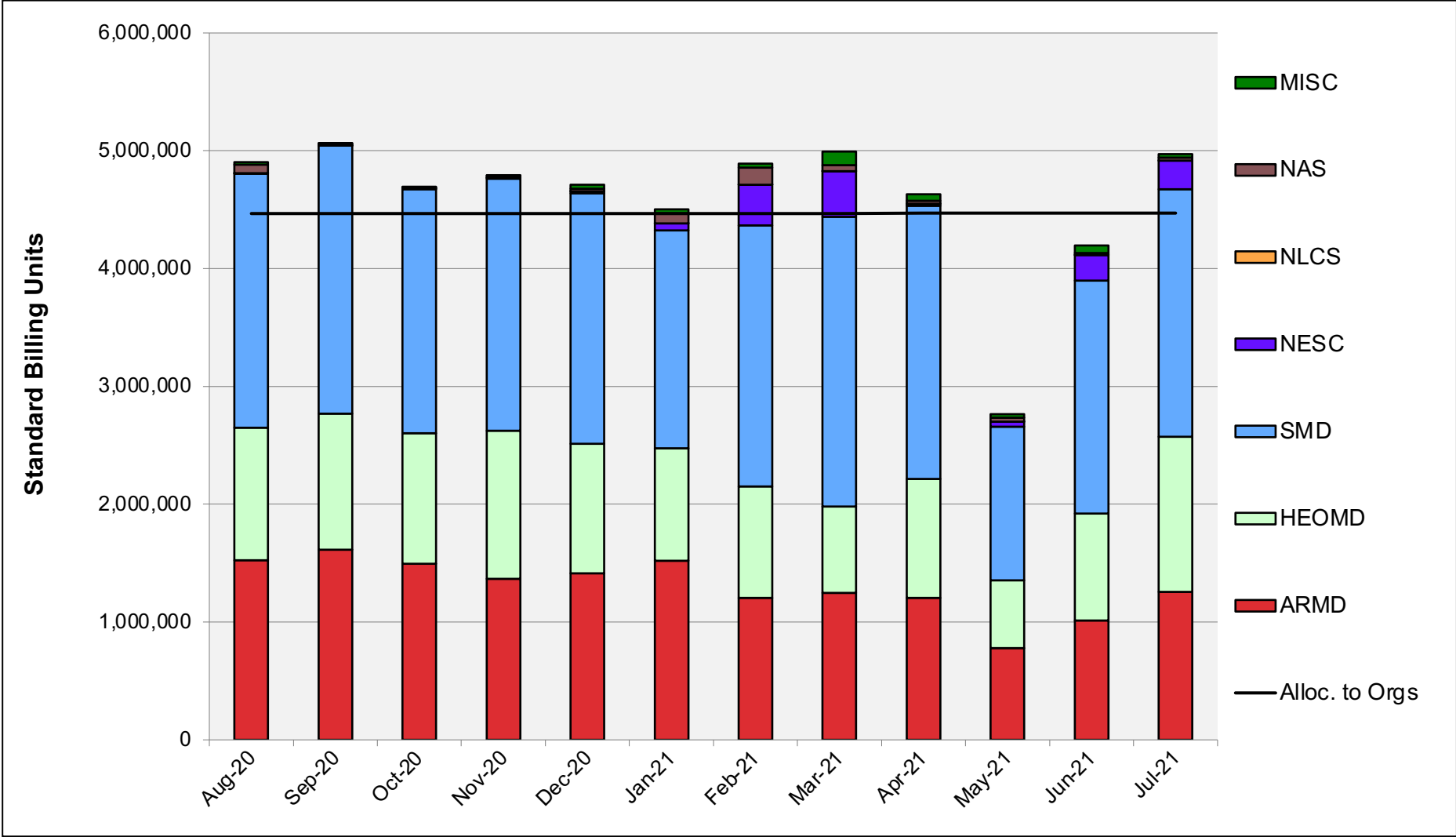
Tape Archive Status



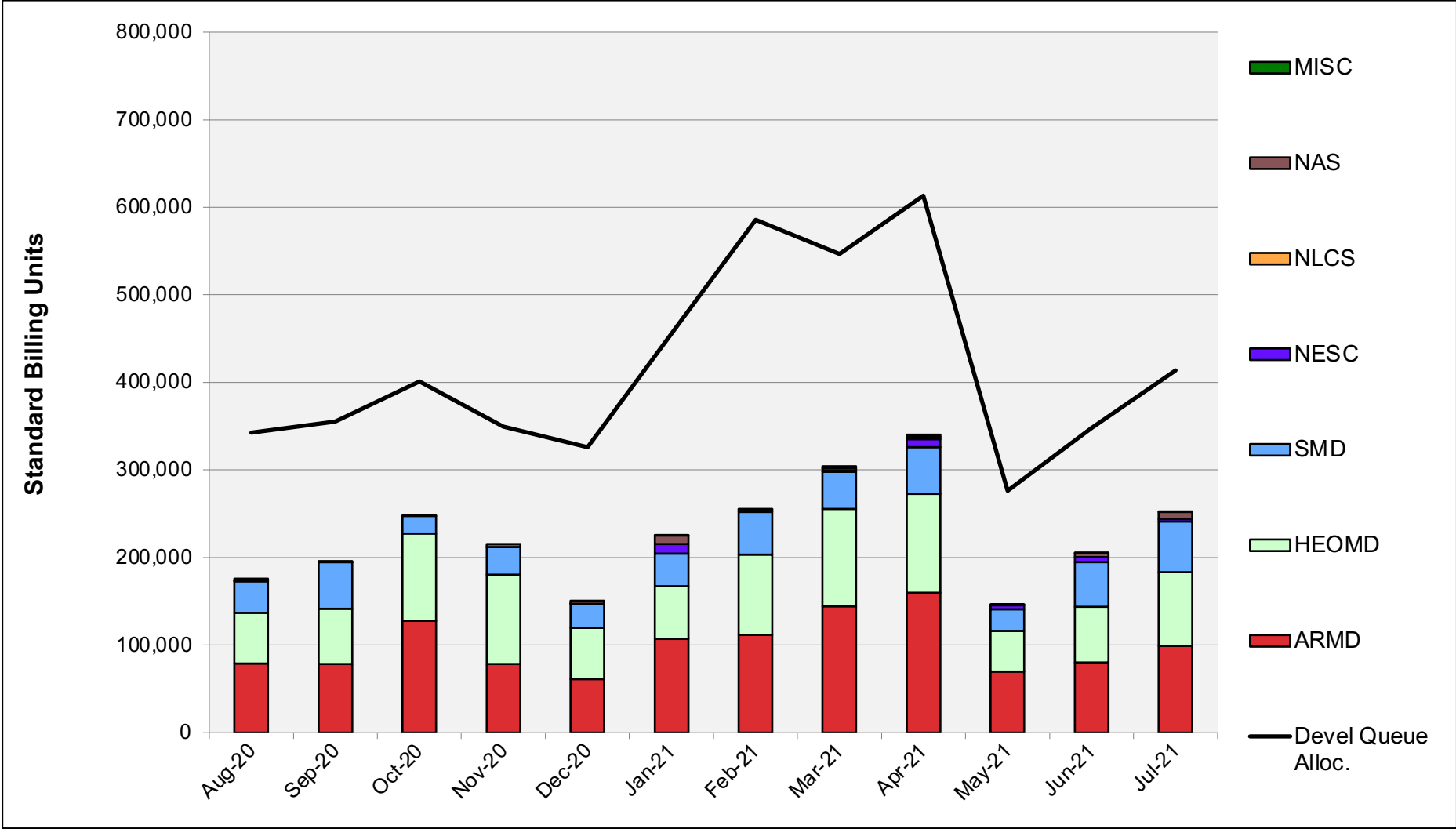
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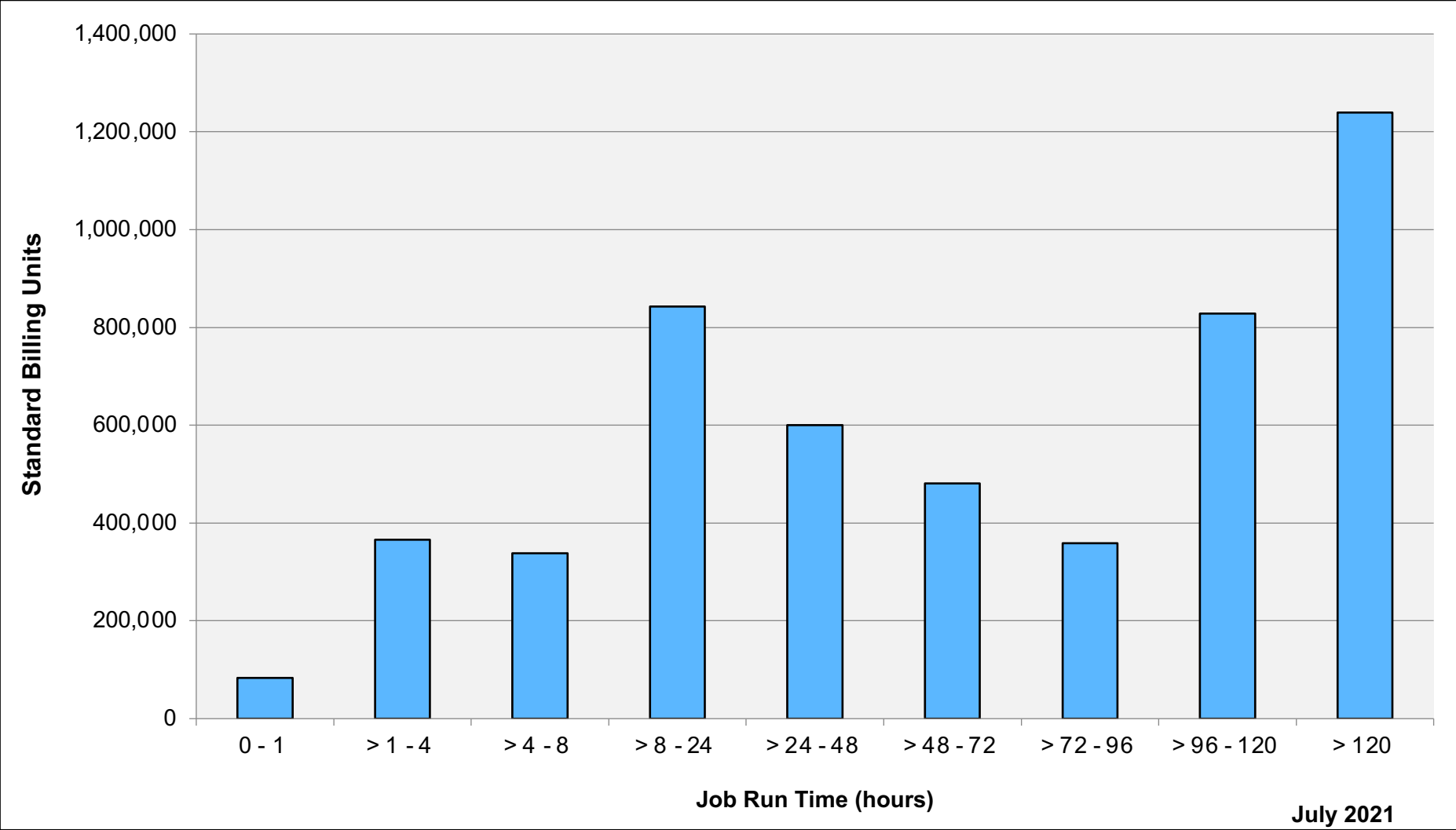
Pleiades: SBUs Reported, Normalized to 30-Day Month



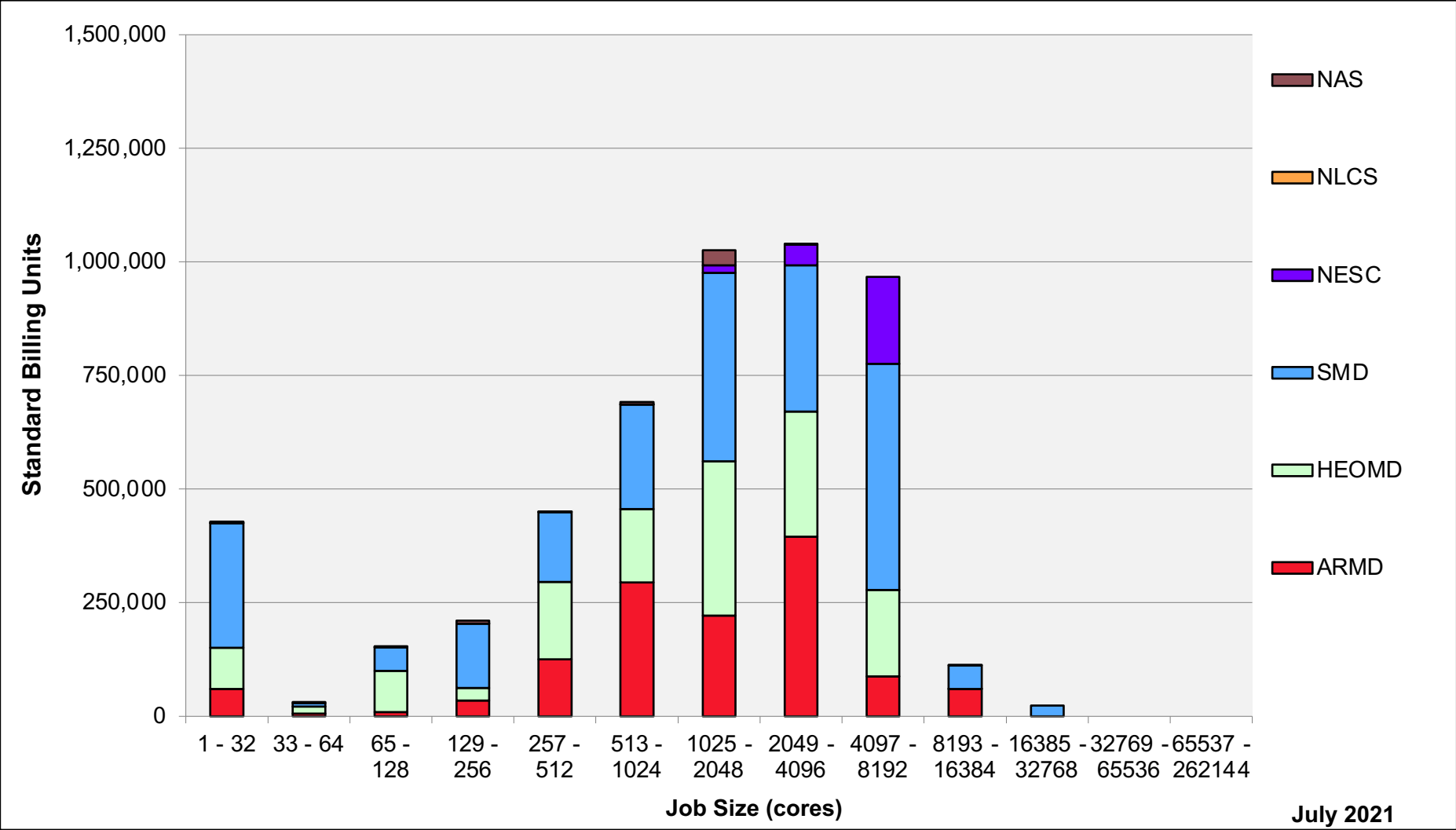
Pleiades: Devel Queue Utilization



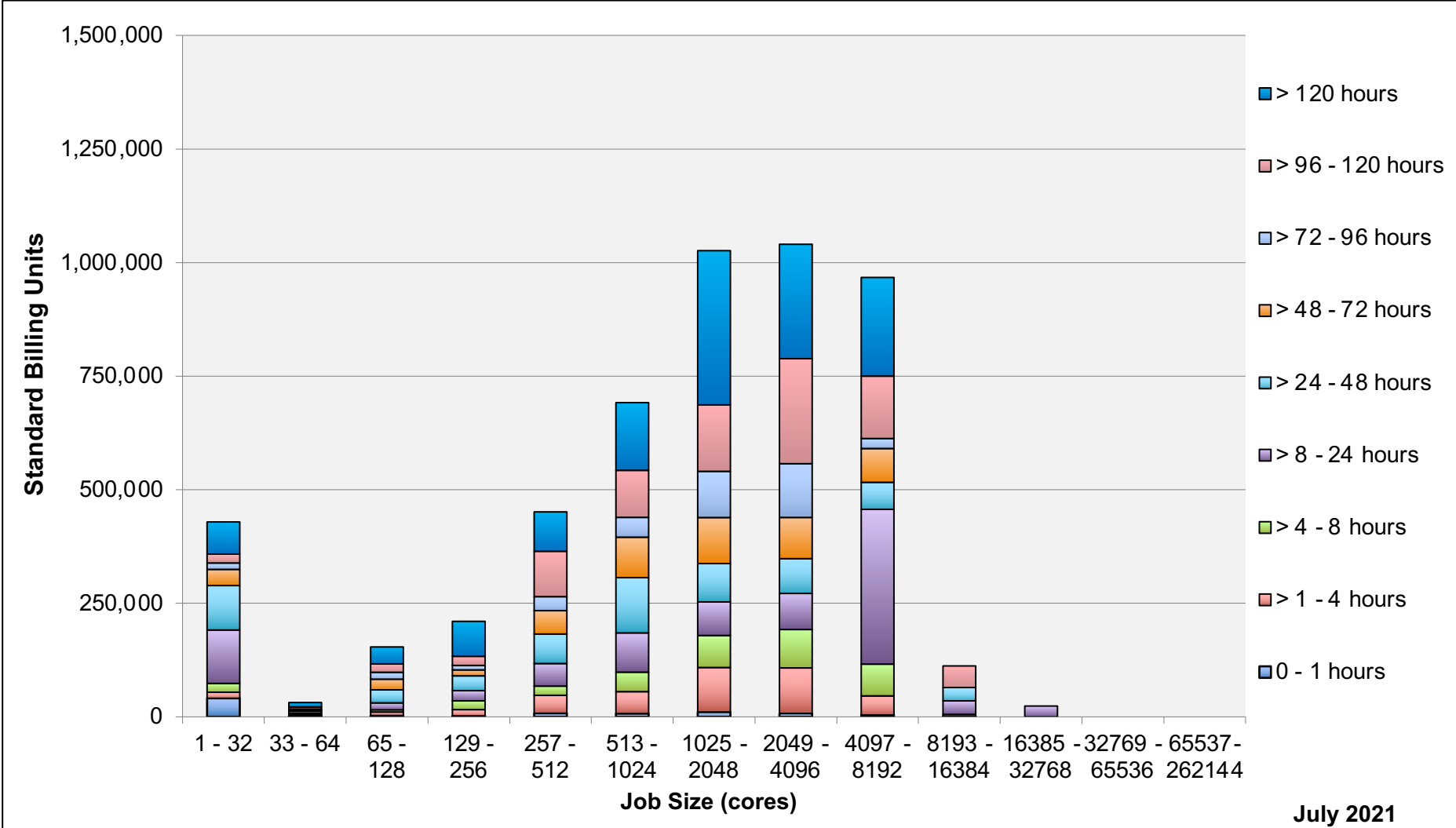
Pleiades: Monthly Utilization by Job Length



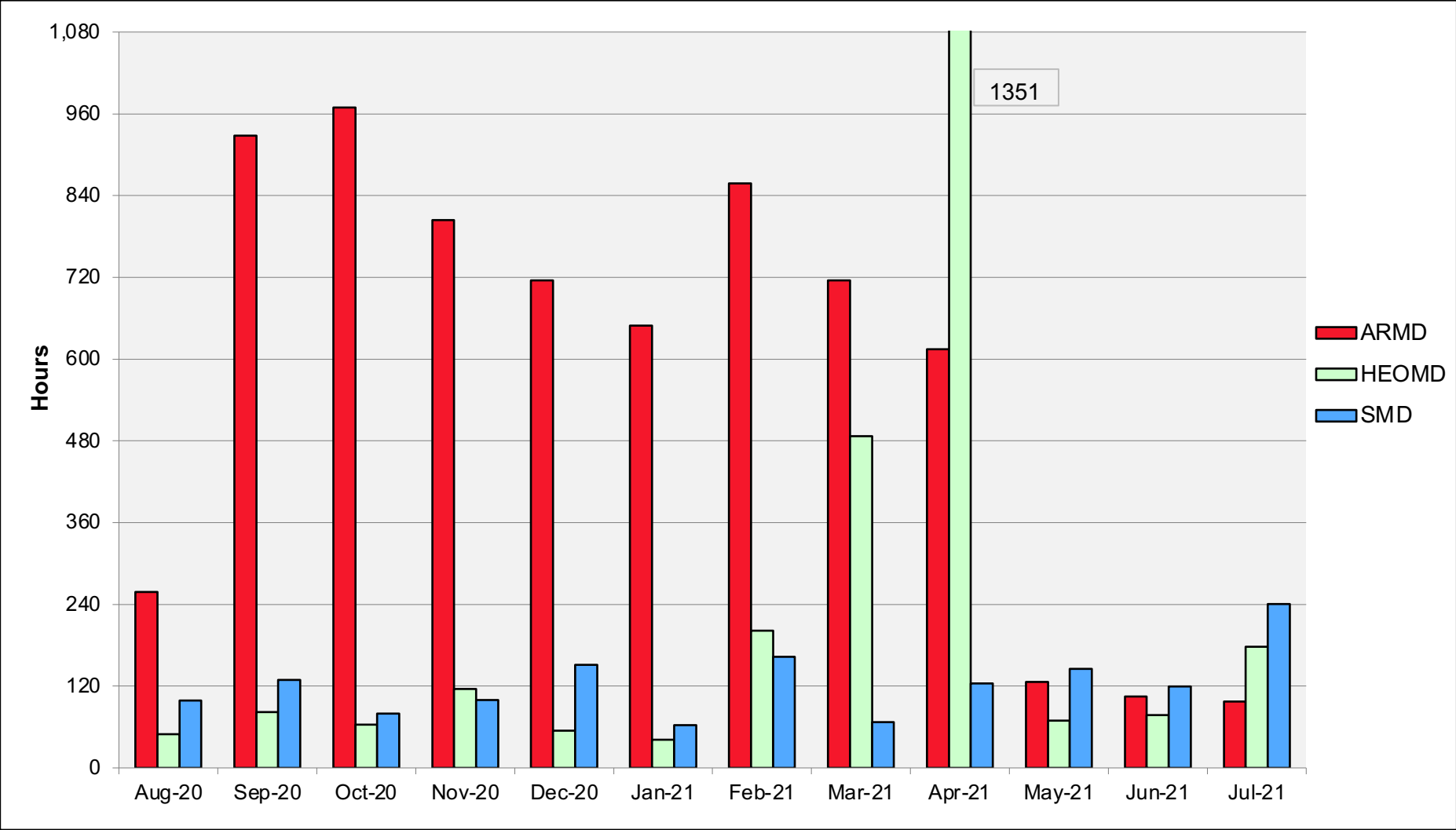
Pleiades: Monthly Utilization by Job Size



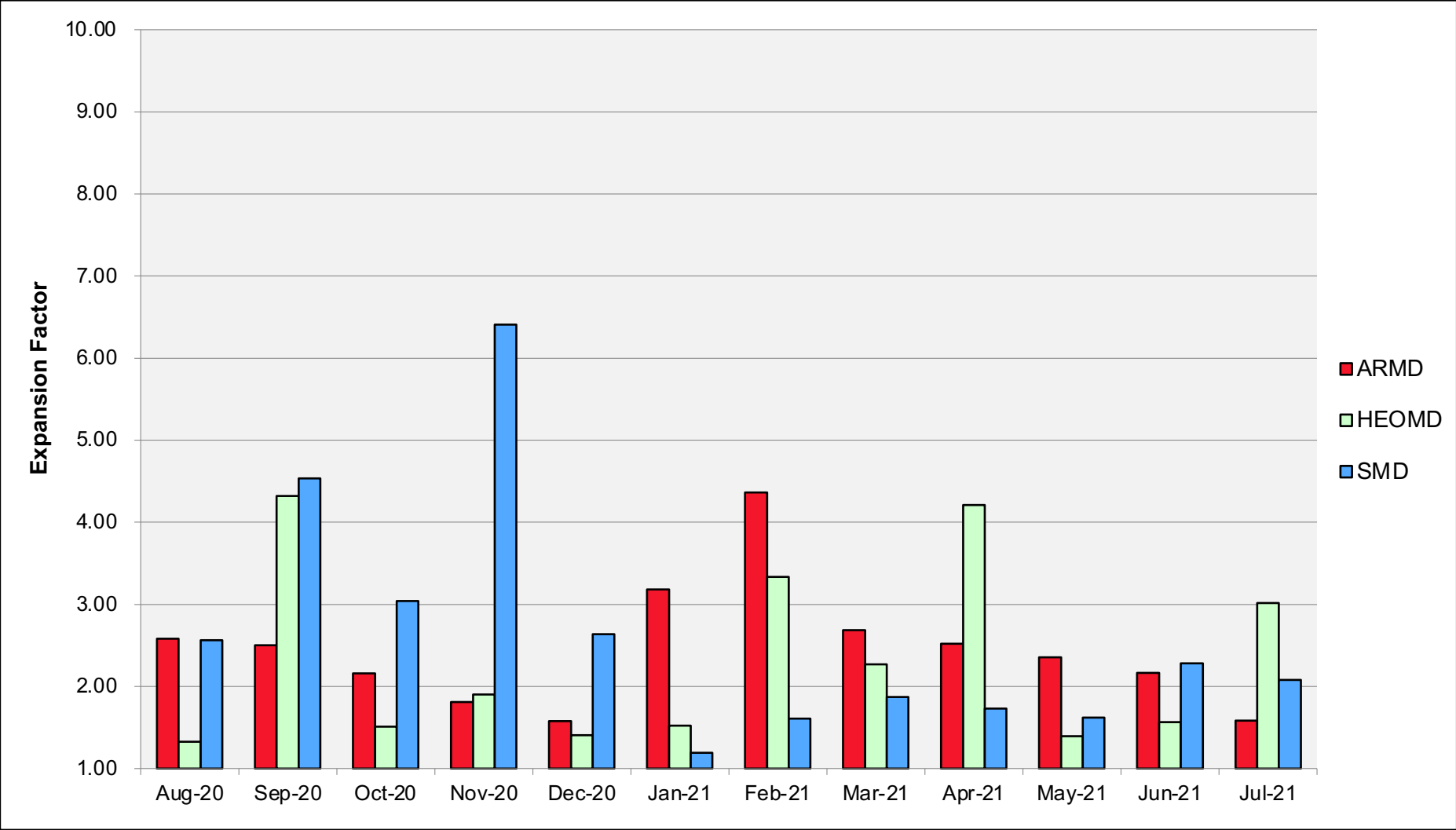
Pleiades: Monthly Utilization by Size and Length



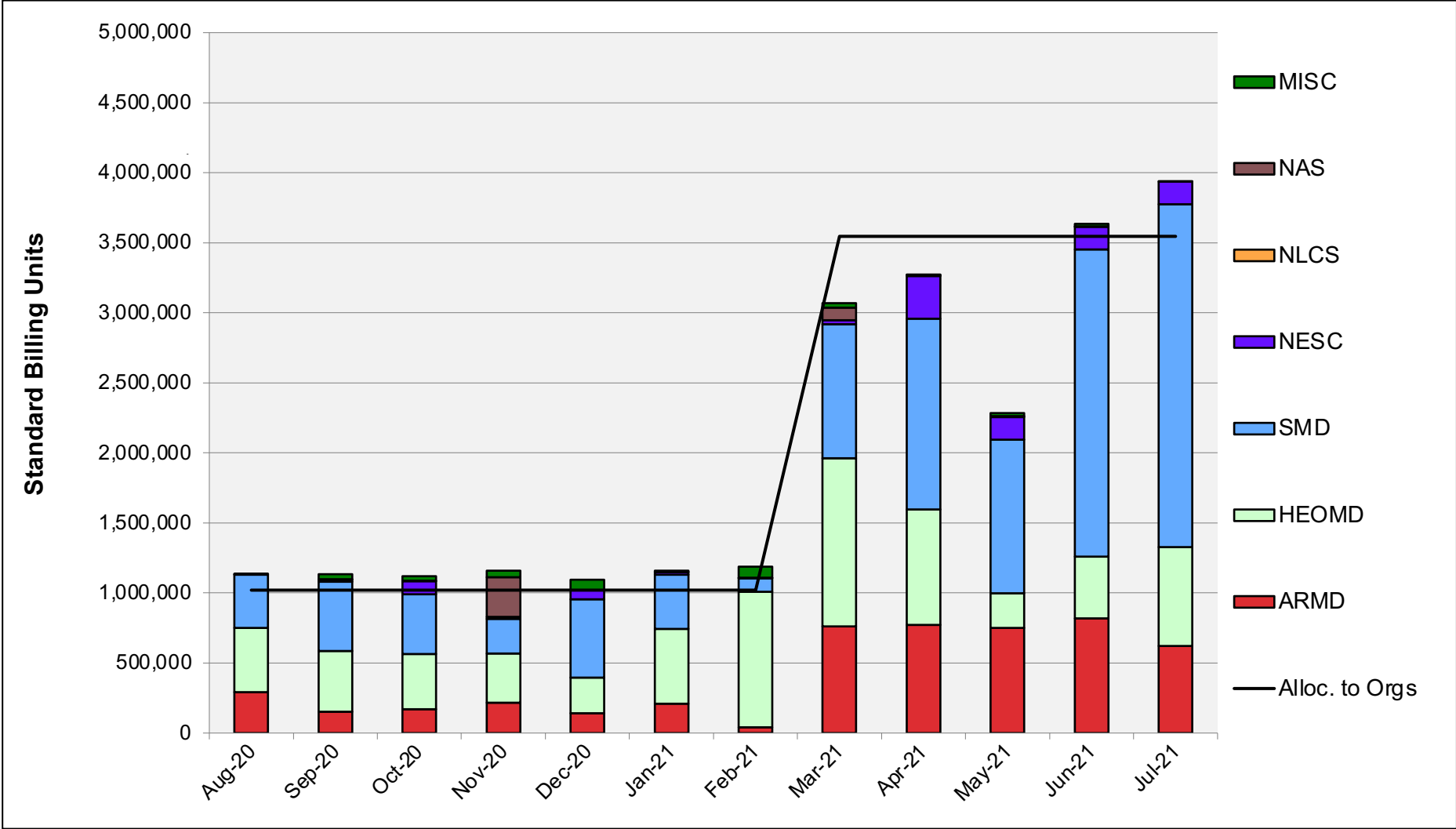
Pleiades: Average Time to Clear All Jobs



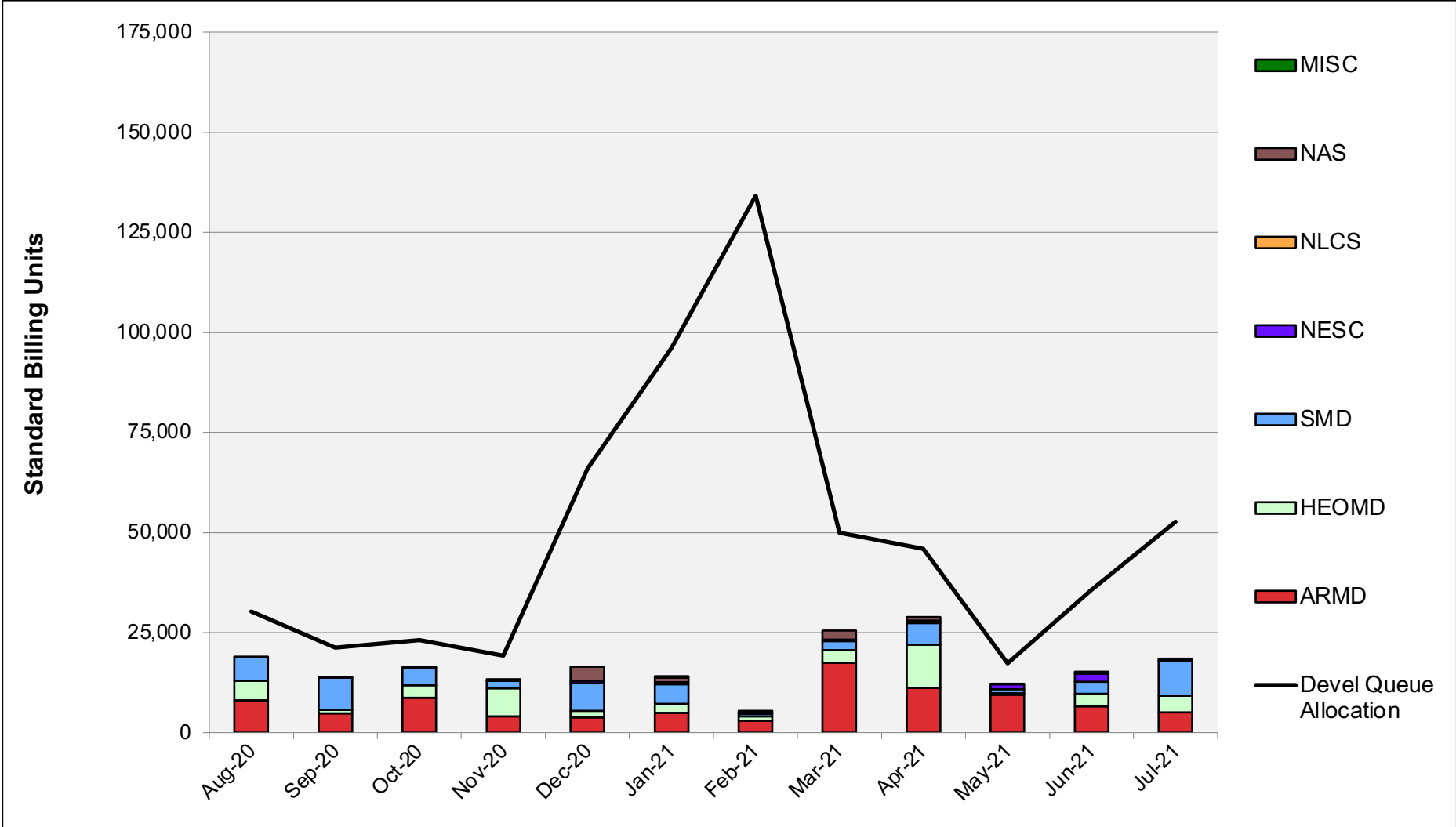
Pleiades: Average Expansion Factor



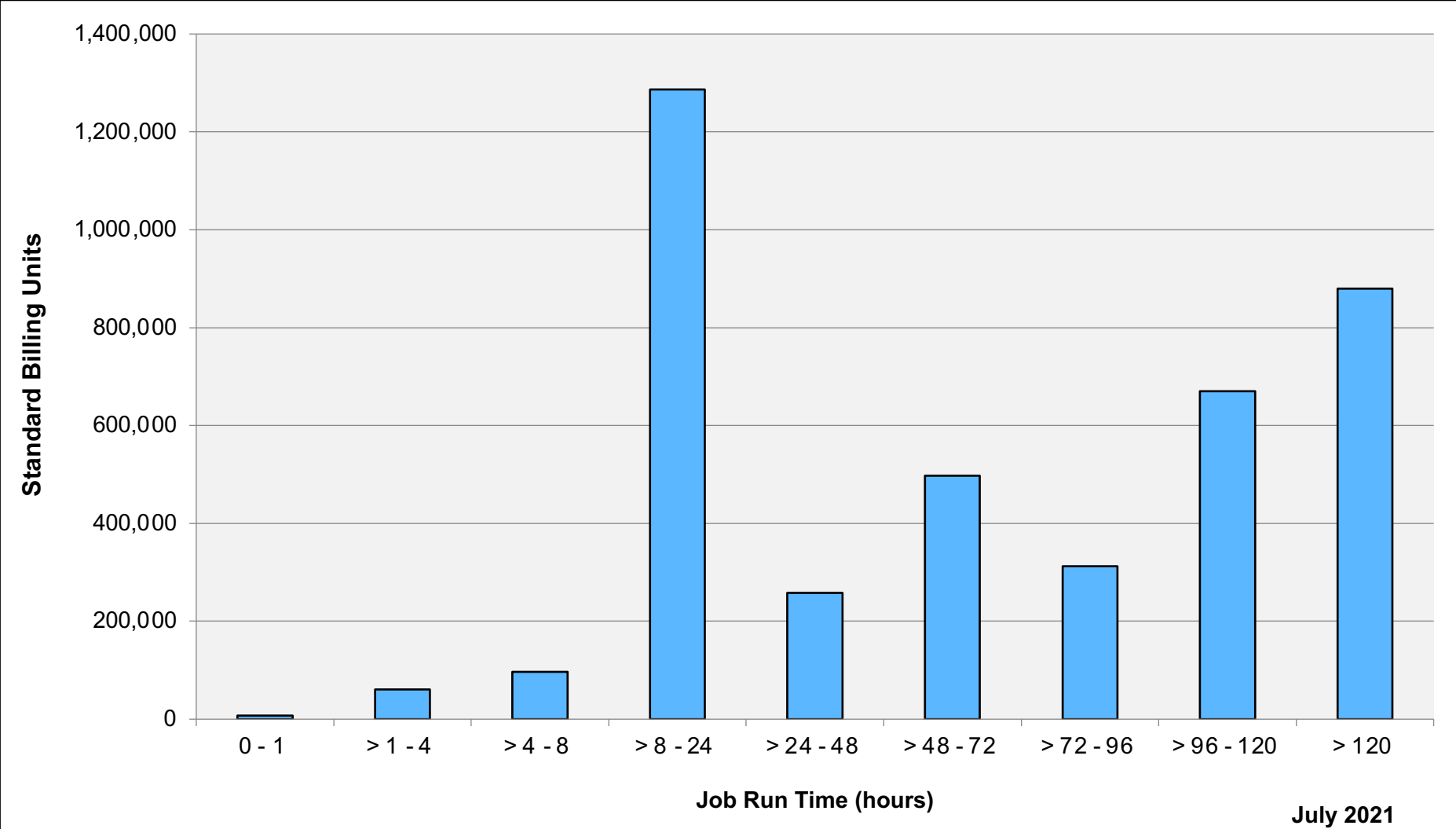
Aitken: SBUs Reported, Normalized to 30-Day Month



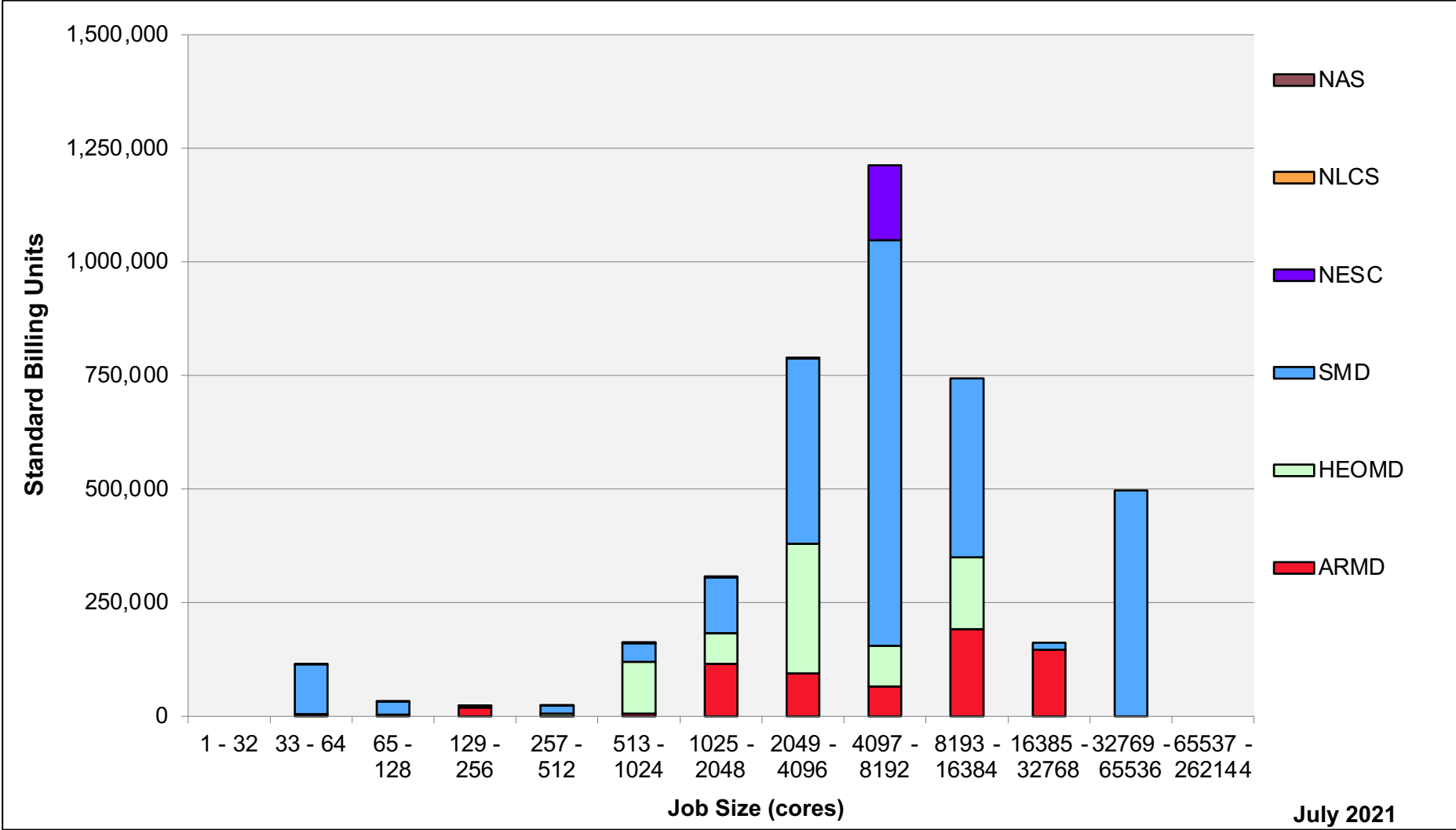
Aitken: Devel Queue Utilization



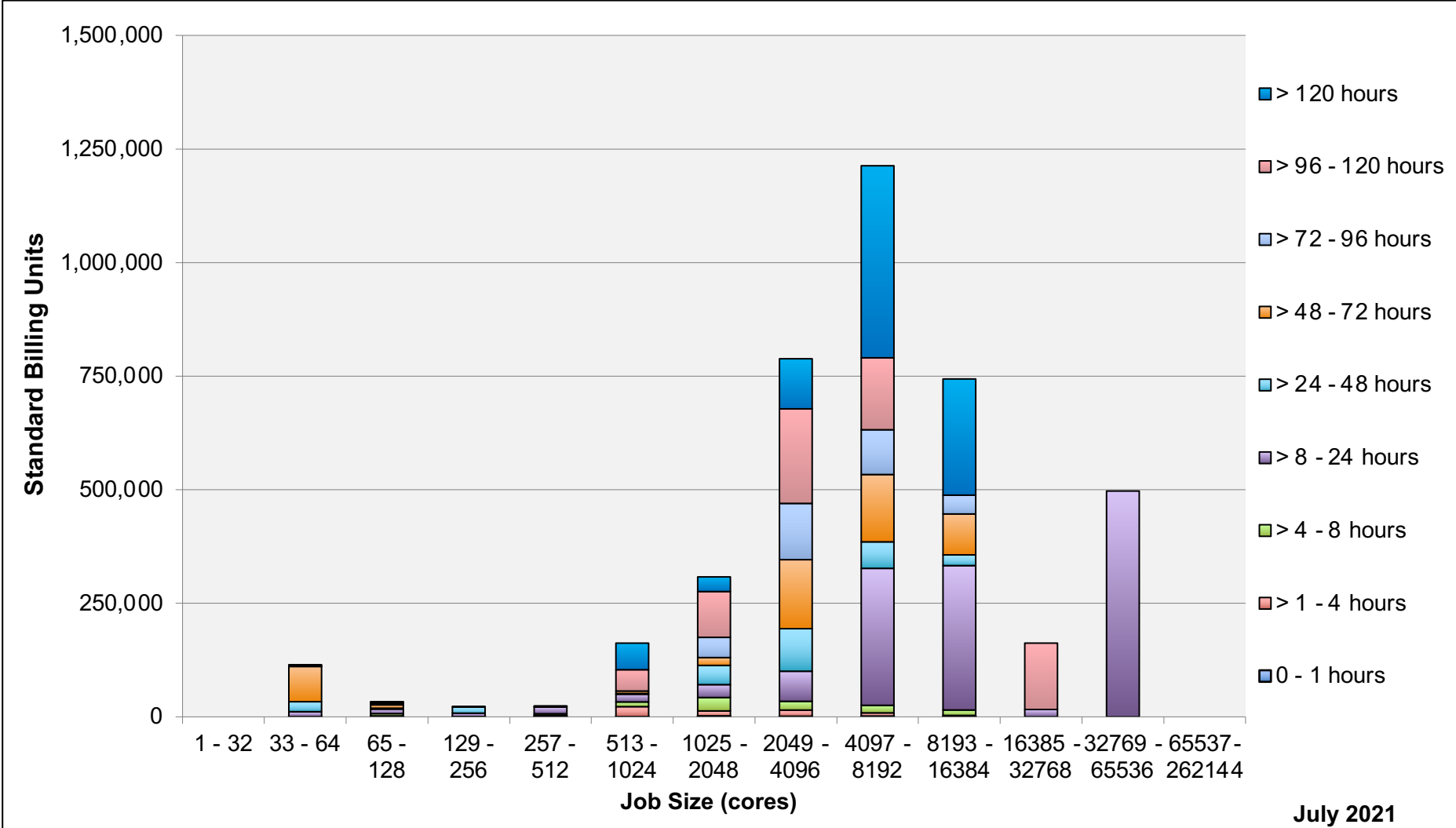
Aitken: Monthly Utilization by Job Length



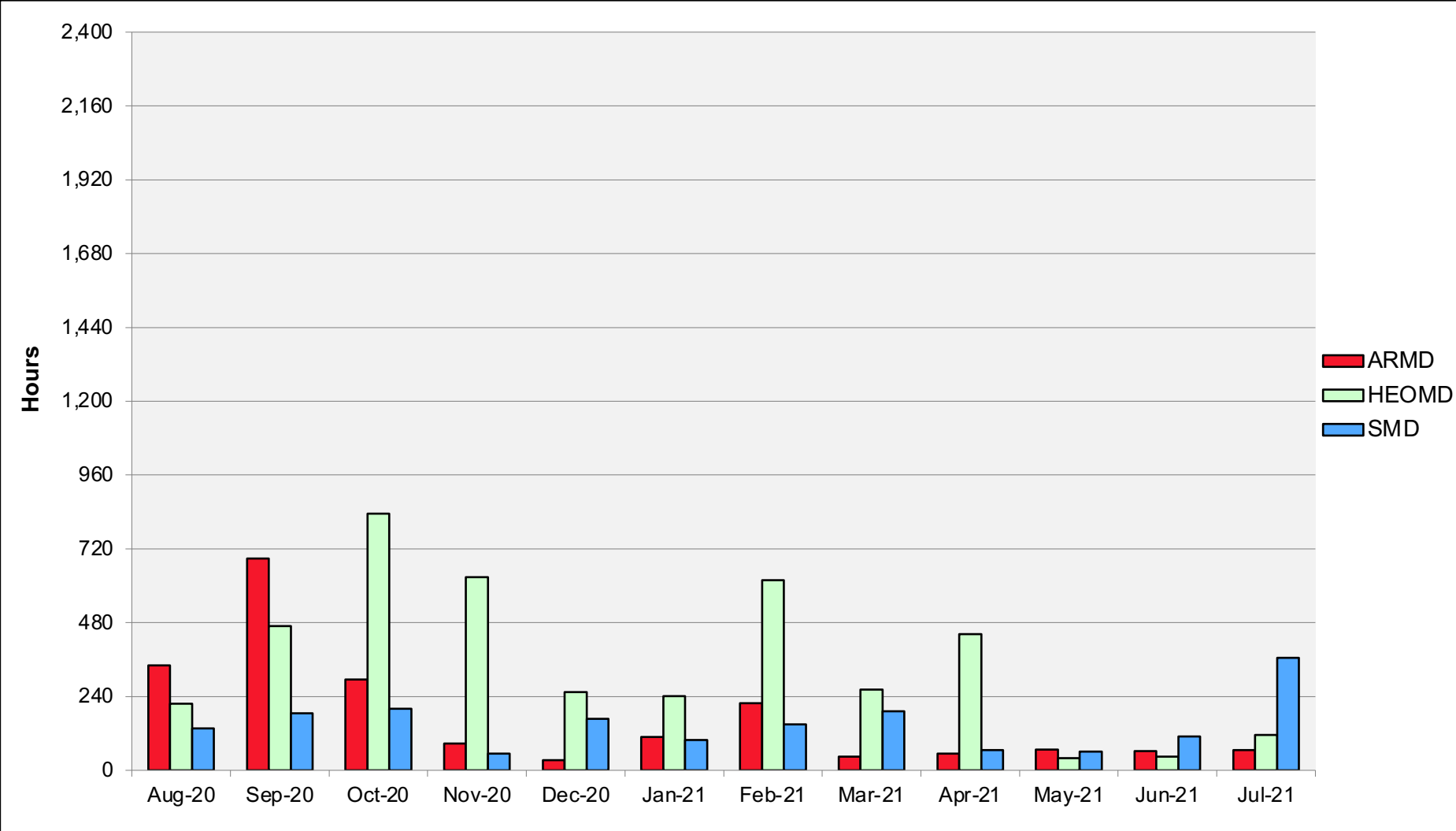
Aitken: Monthly Utilization by Job Size



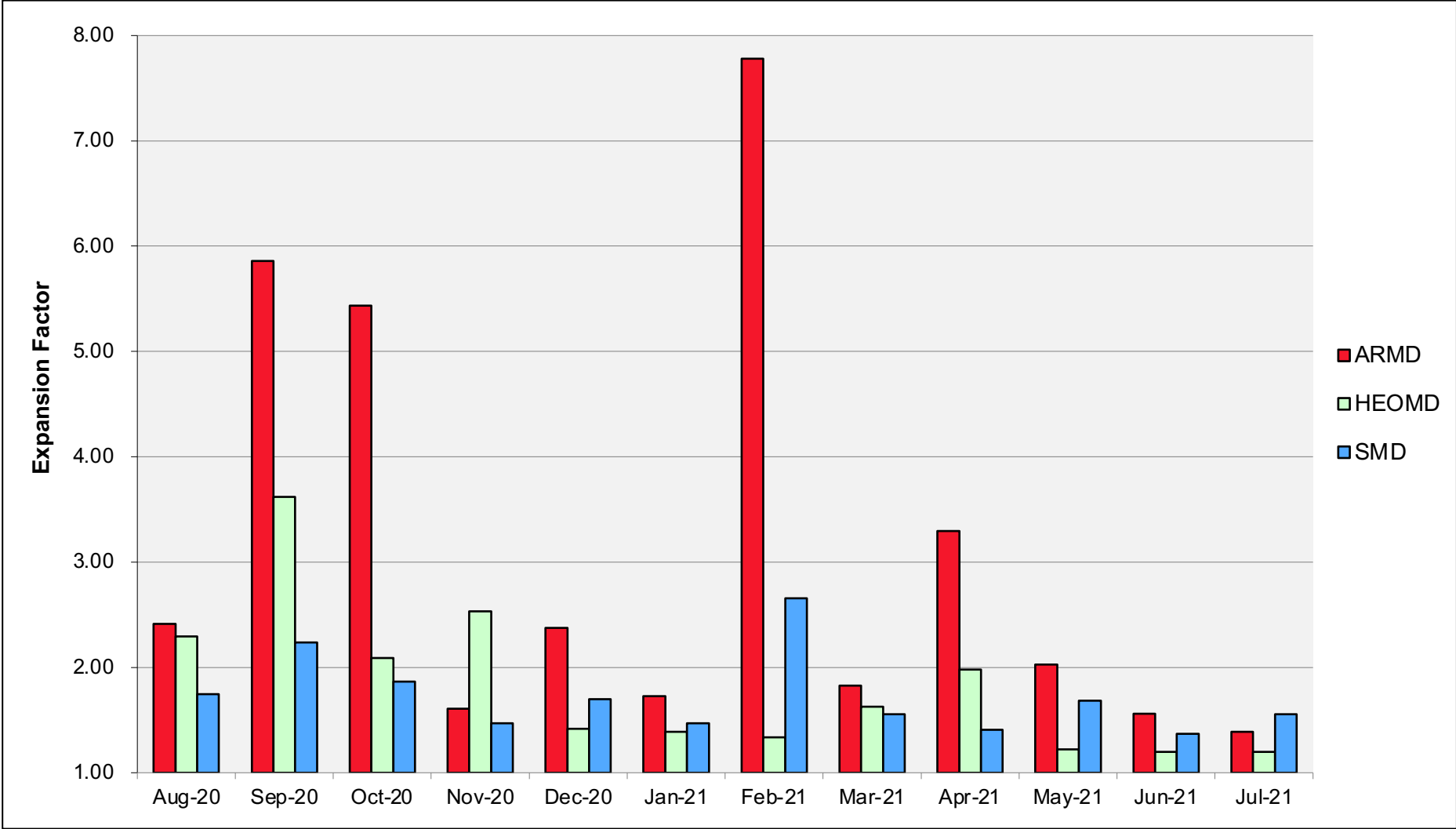
Aitken: Monthly Utilization by Size and Length



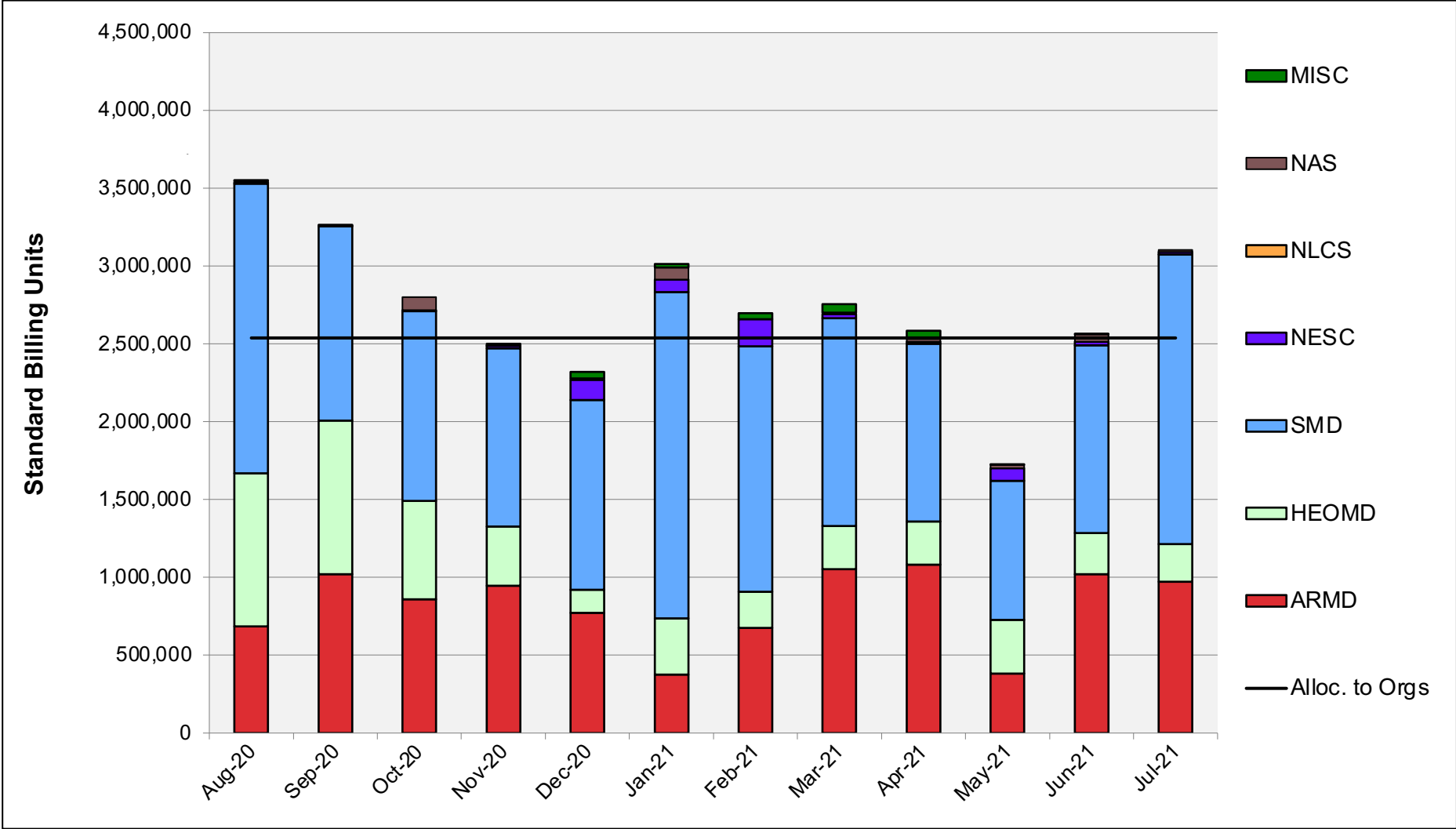
Aitken: Average Time to Clear All Jobs



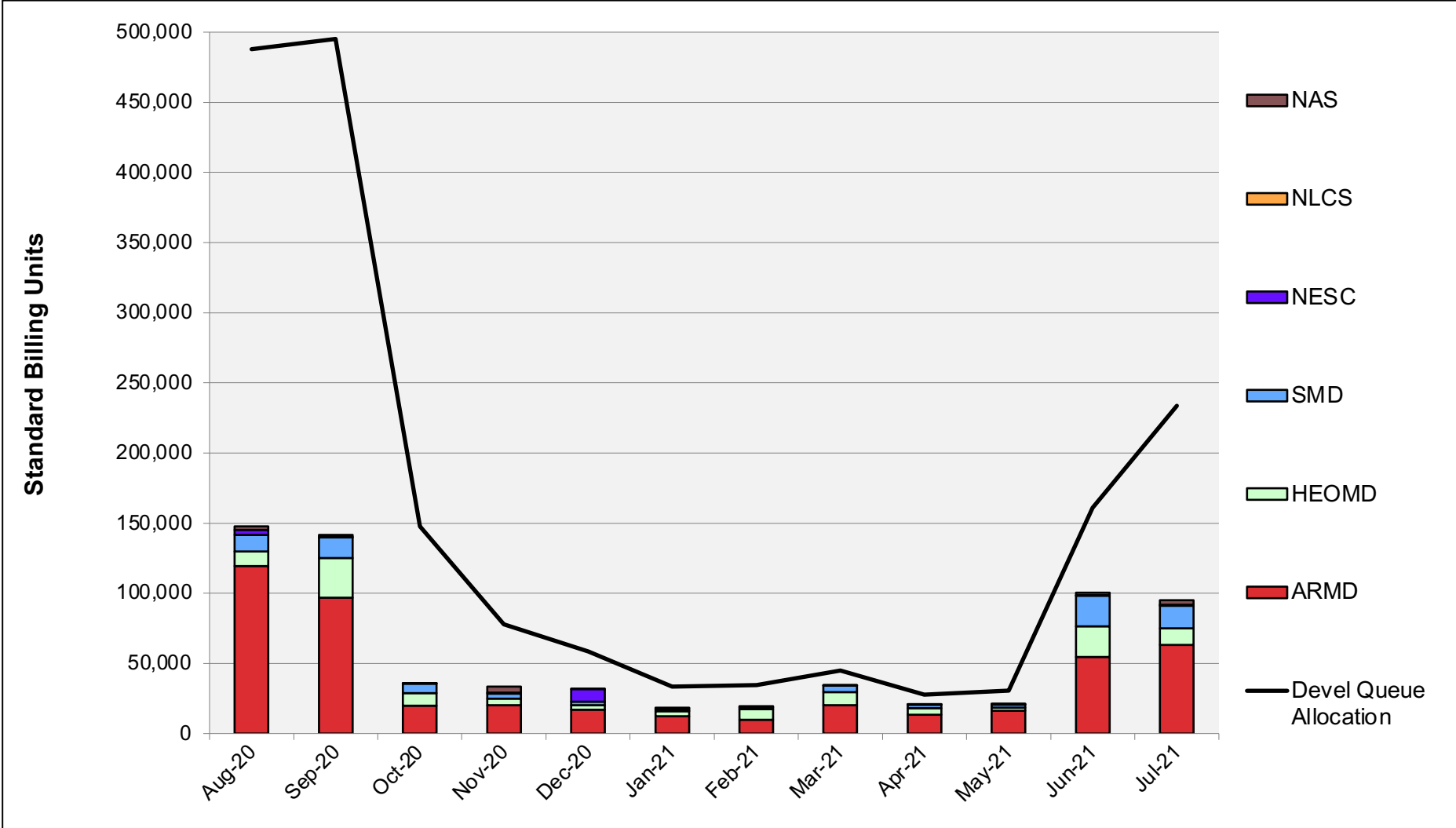
Aitken: Average Expansion Factor



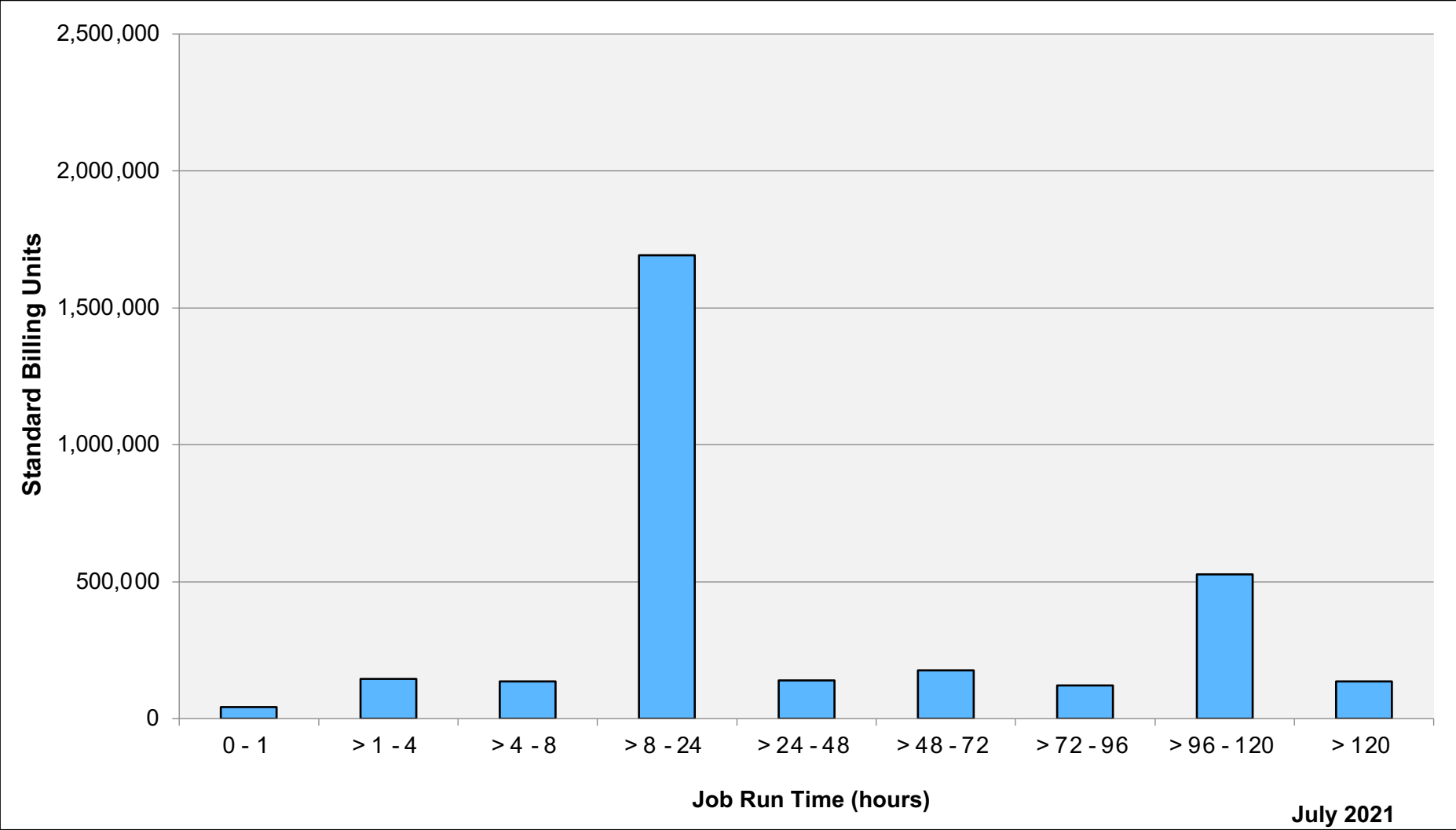
Electra: SBUs Reported, Normalized to 30-Day Month



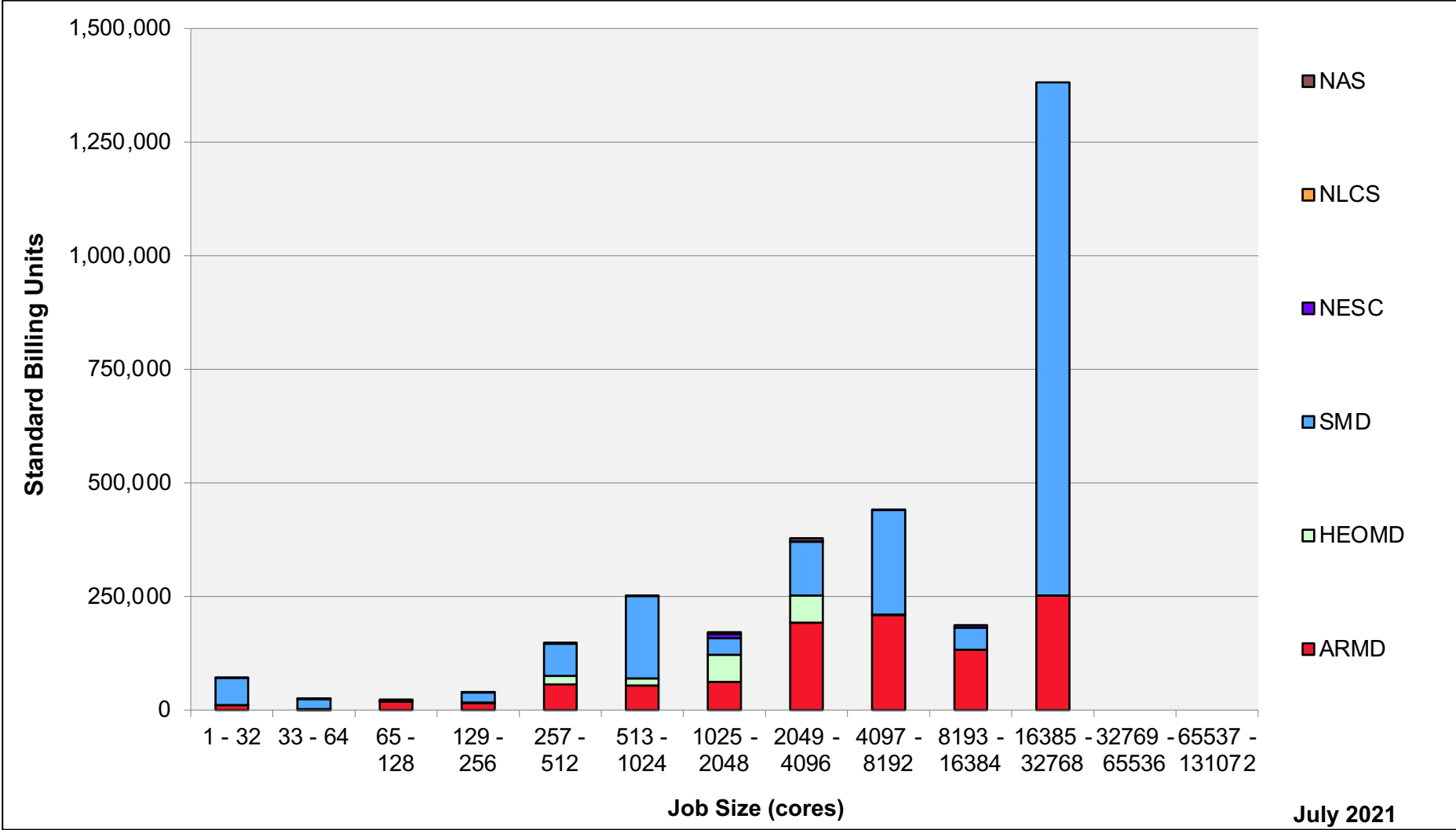
Electra: Devel Queue Utilization



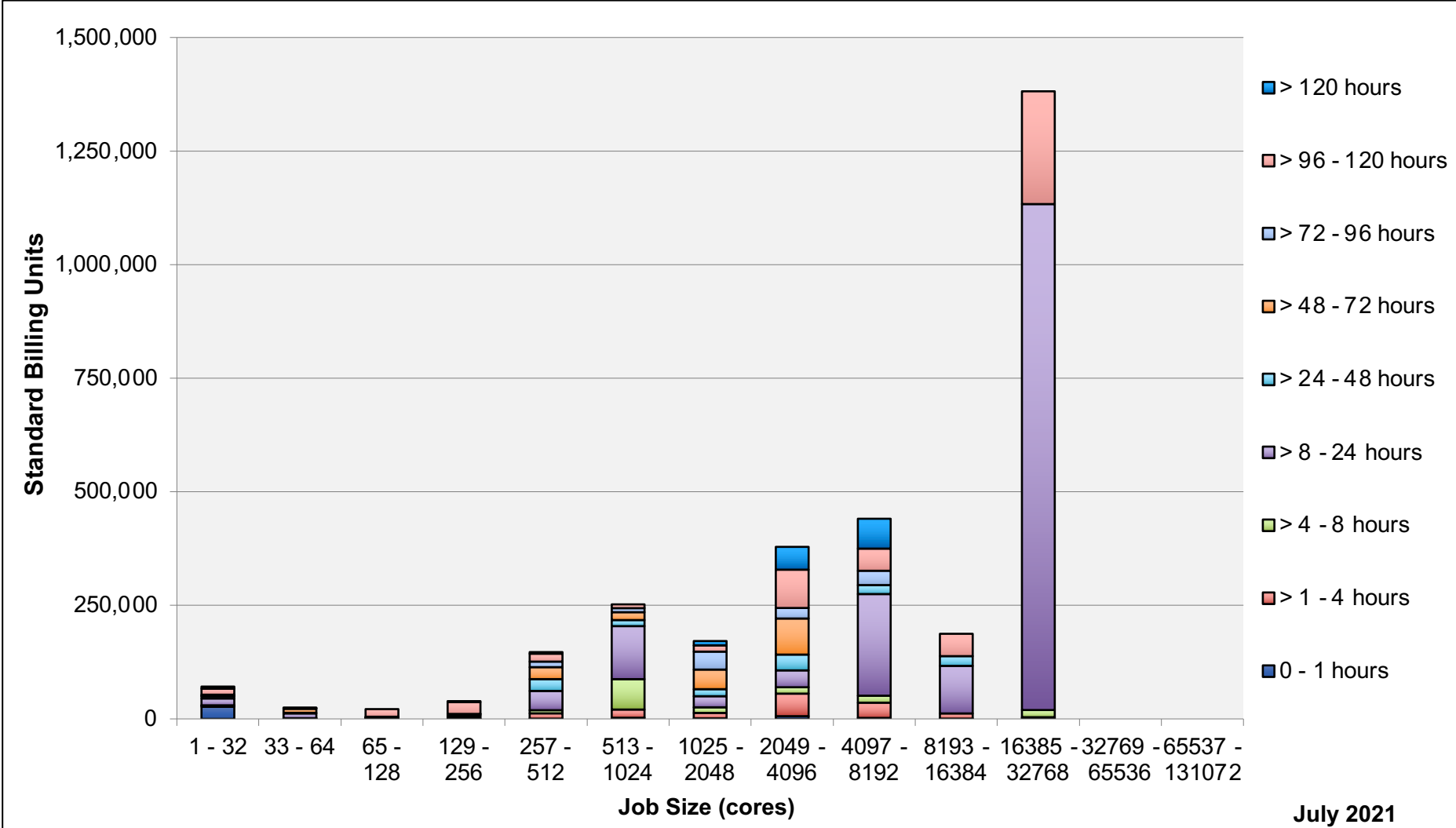
Electra: Monthly Utilization by Job Length



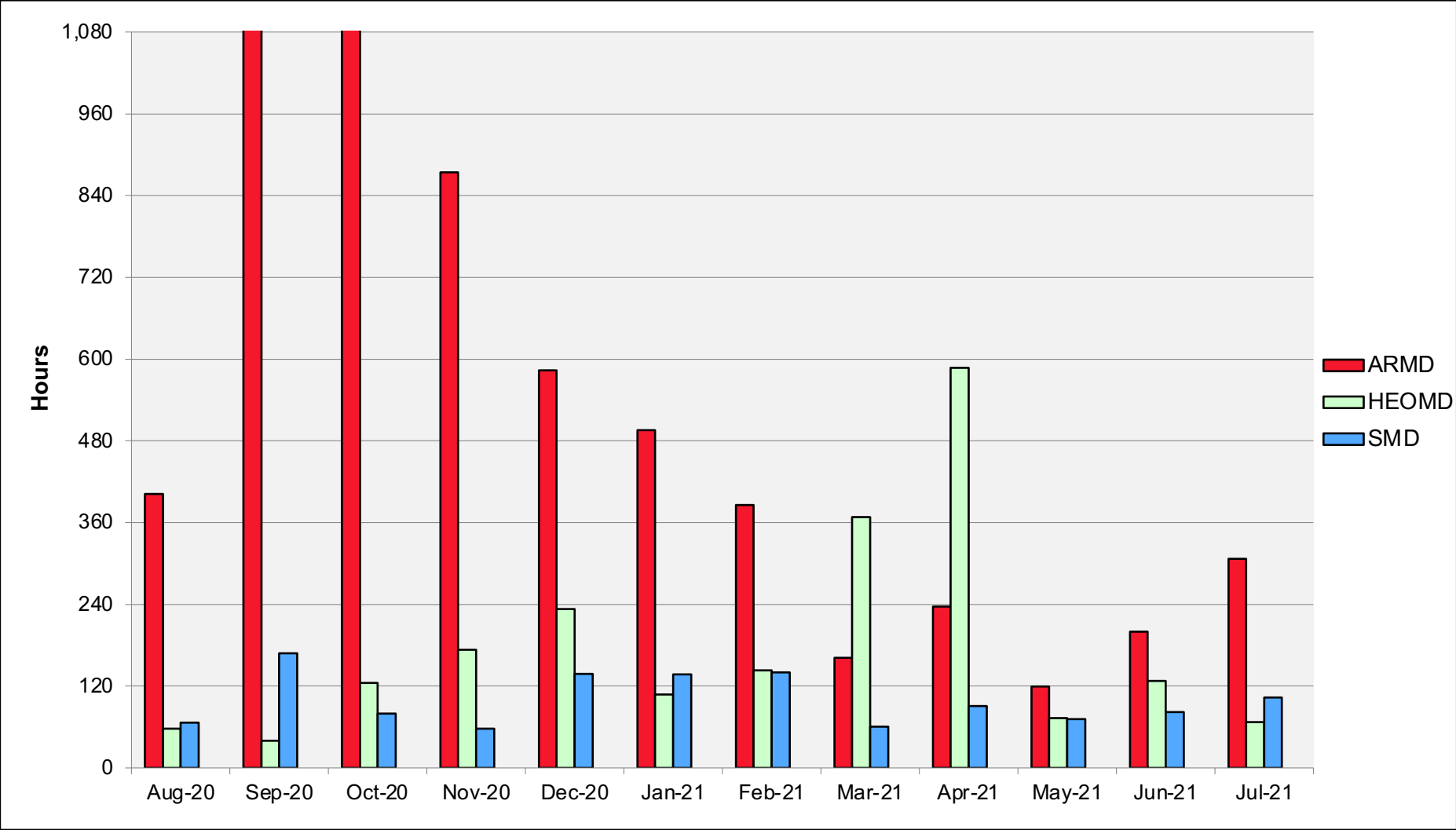
Electra: Monthly Utilization by Job Size



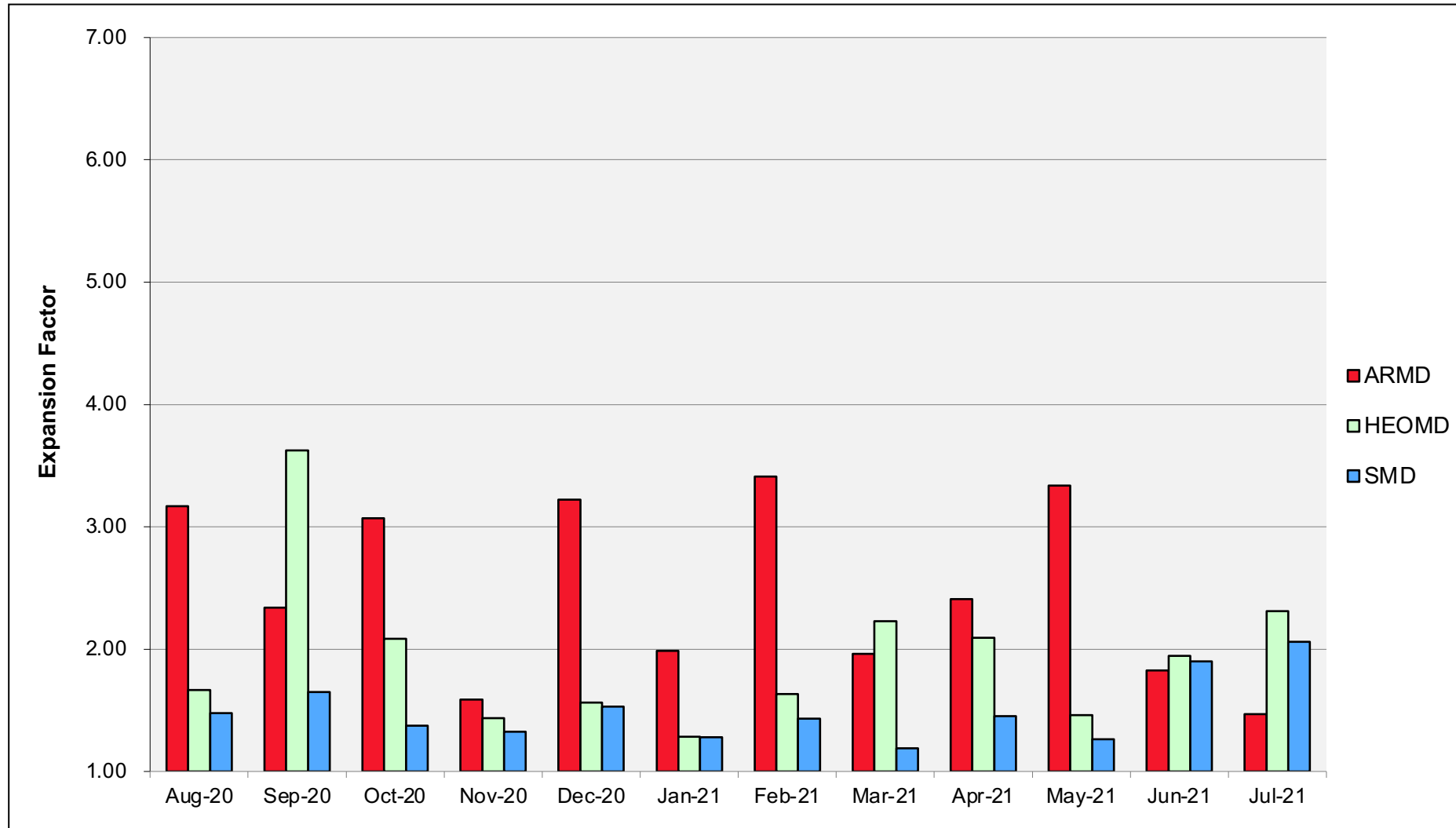
Electra: Monthly Utilization by Size and Length



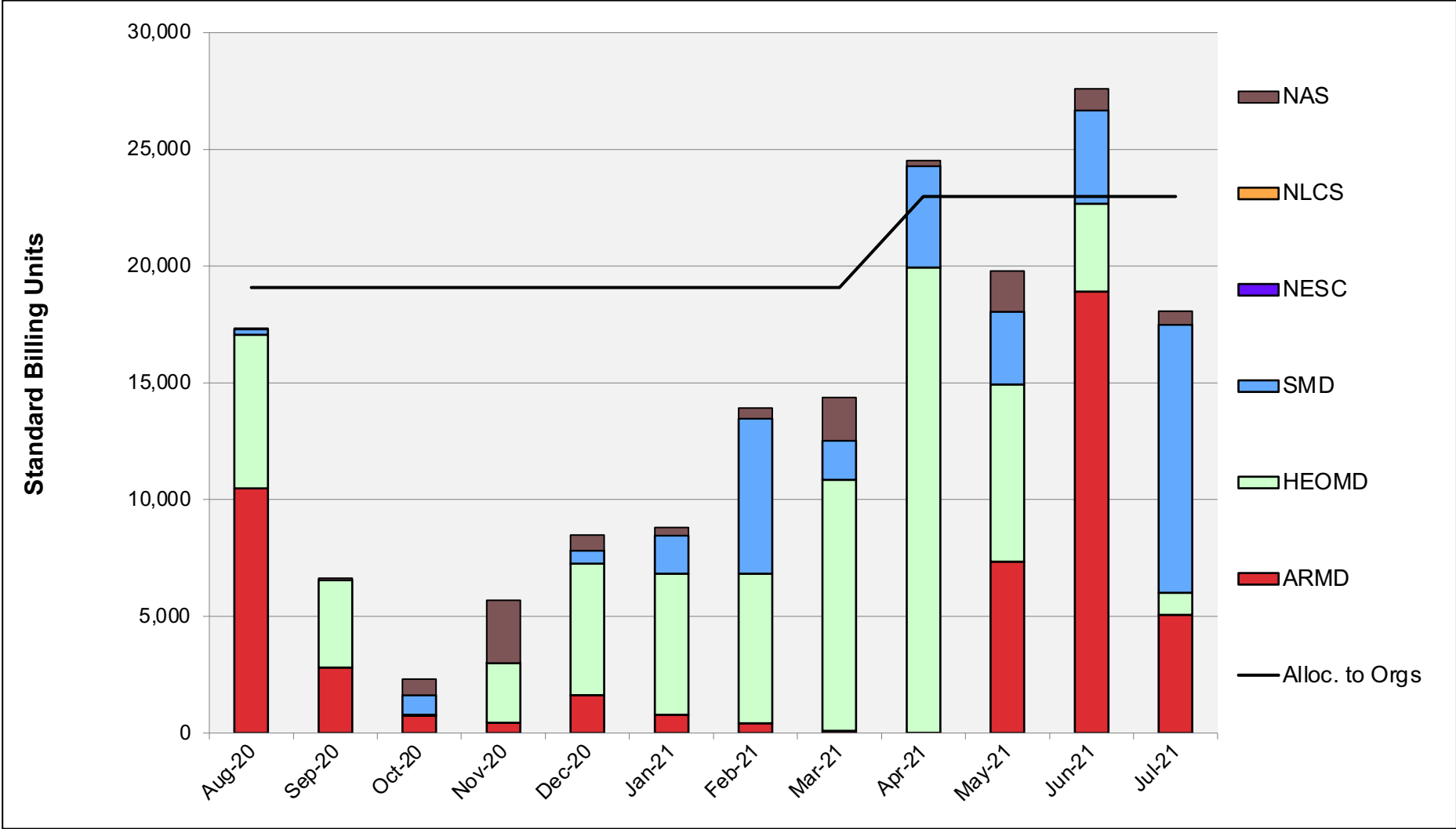
Electra: Average Time to Clear All Jobs



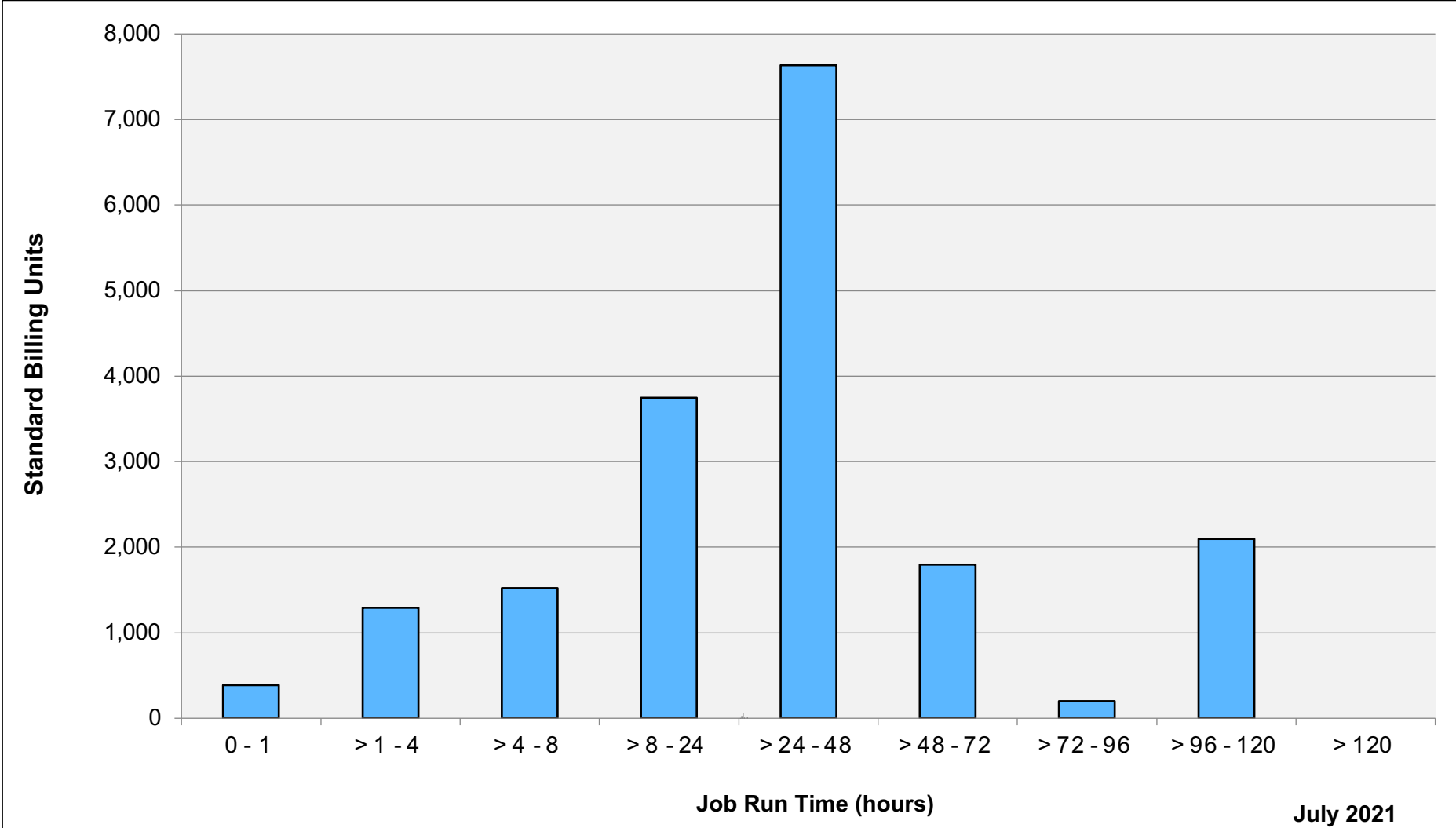
Electra: Average Expansion Factor



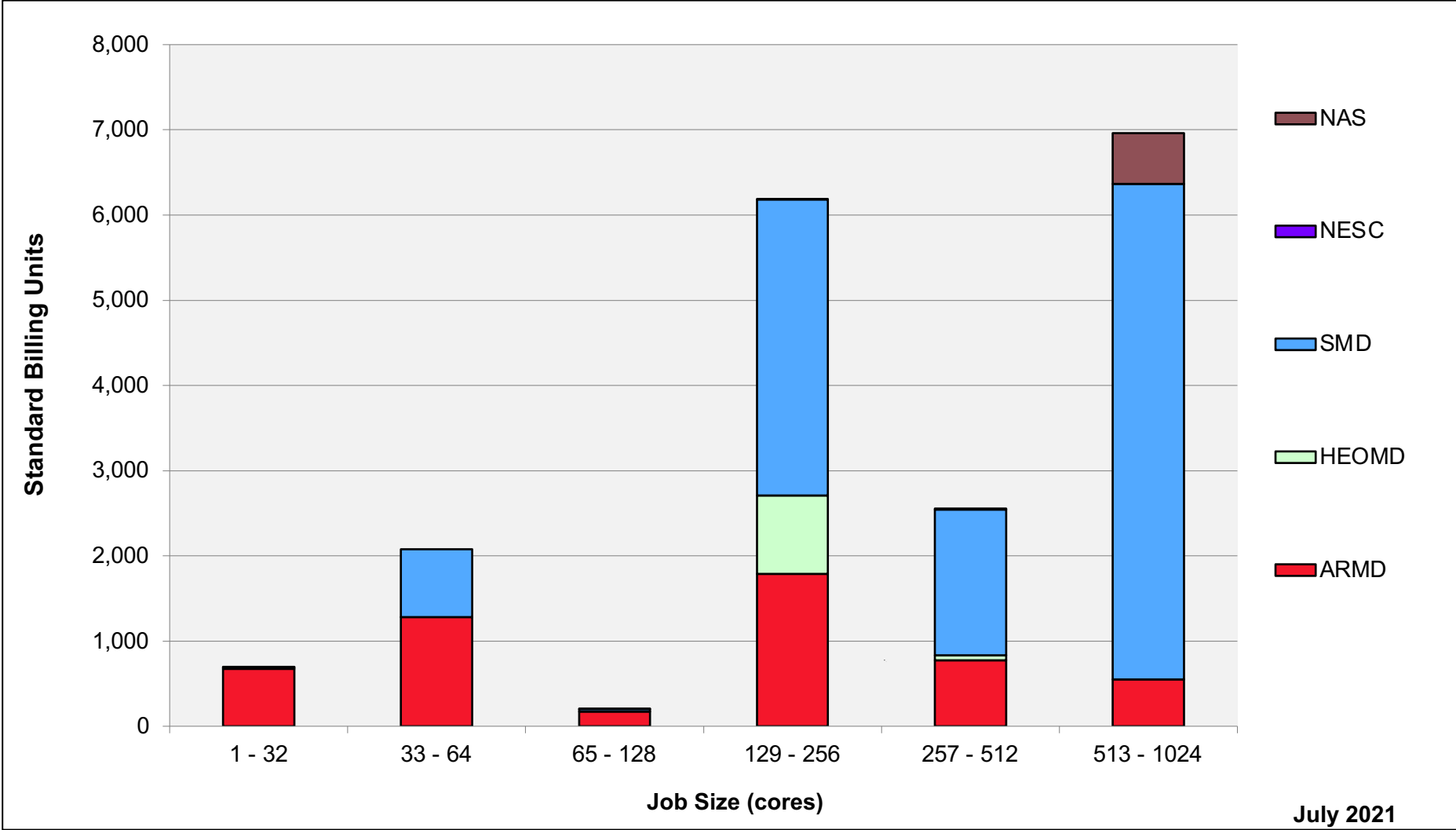
Endeavour: SBUs Reported, Normalized to 30-Day Month



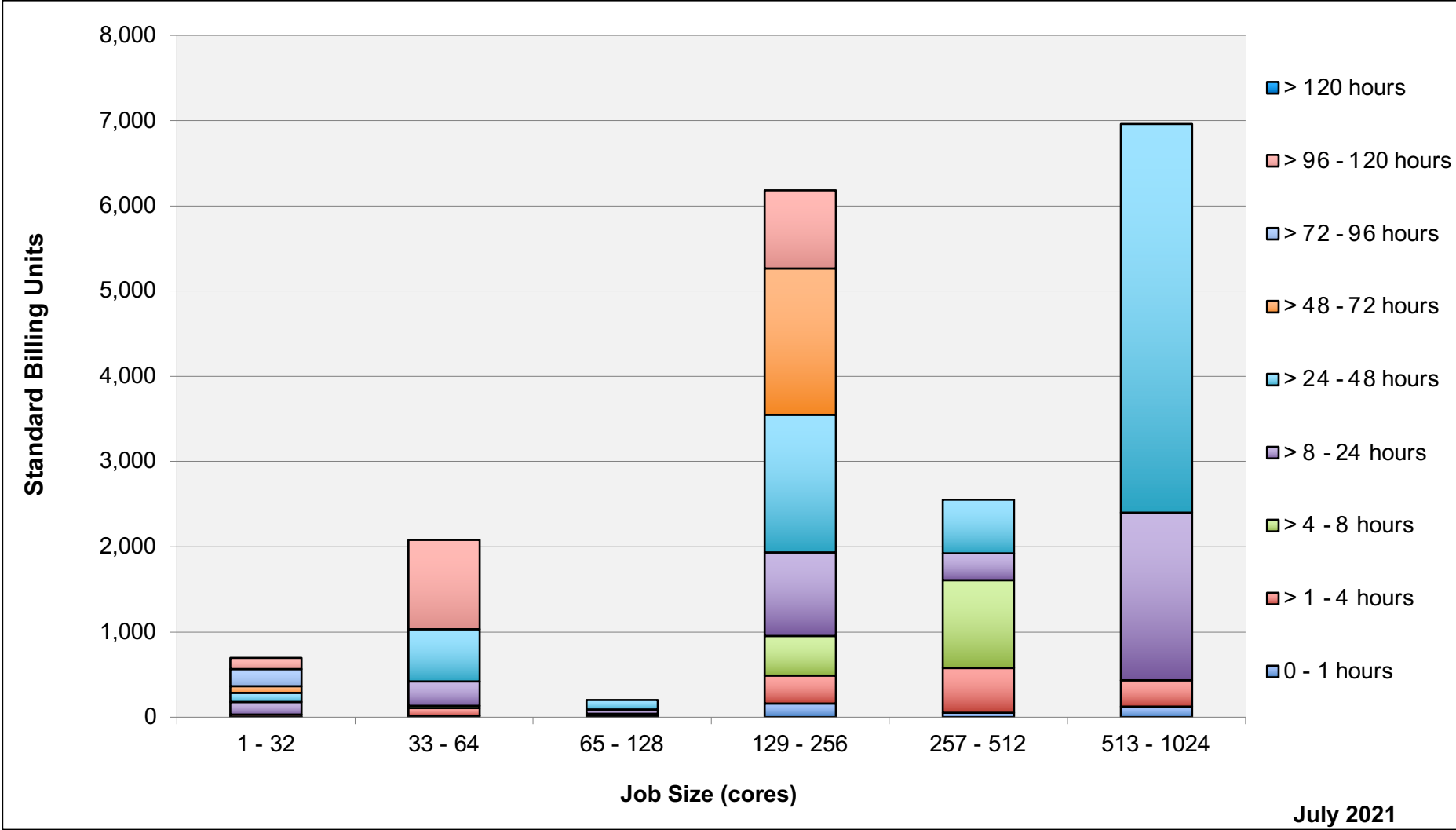
Endeavour: Monthly Utilization by Job Length



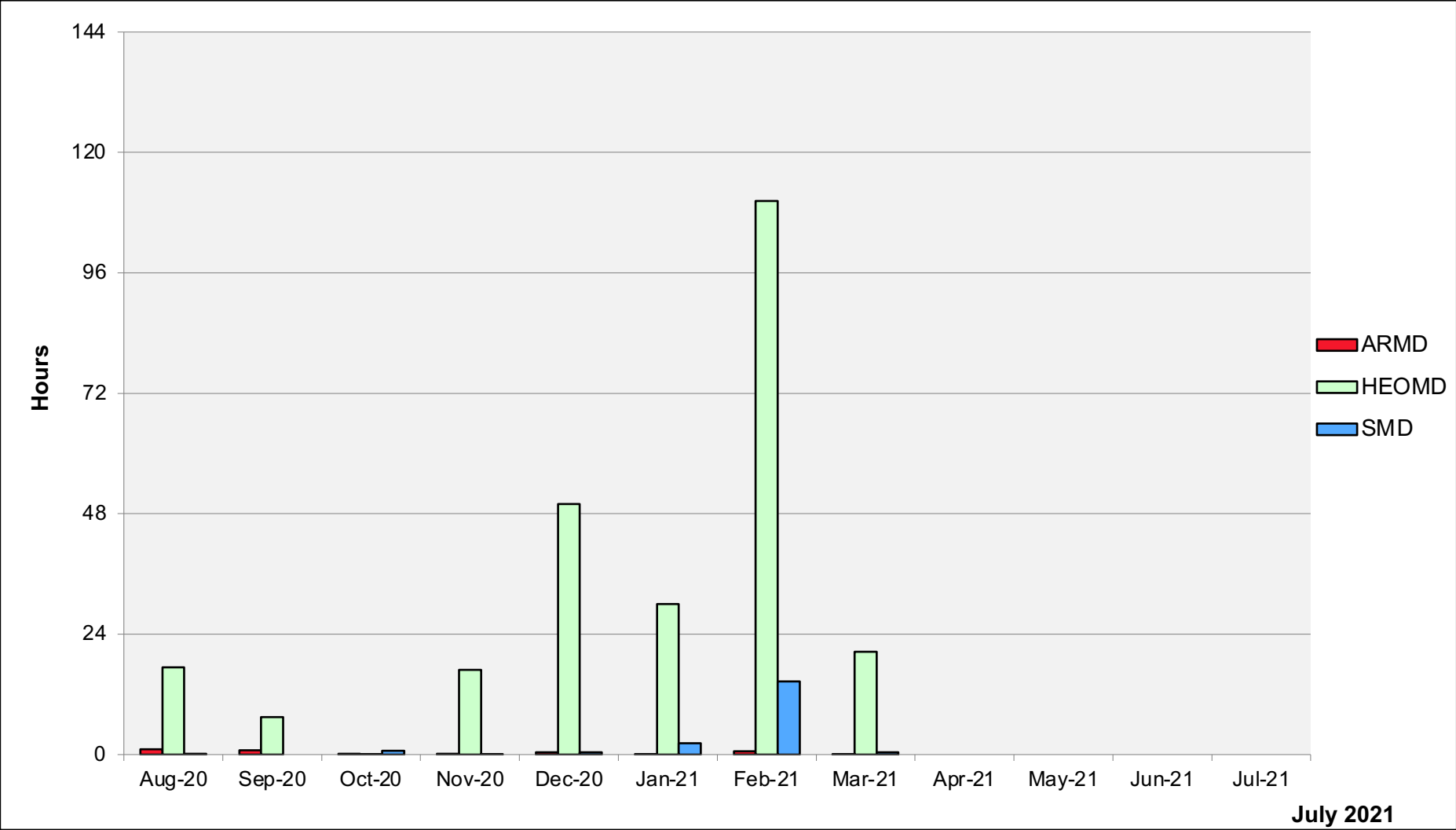
Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor

